

=> d his

(FILE 'HOME' ENTERED AT 16:52:13 ON 03 SEP 2007)

FILE 'REGISTRY' ENTERED AT 16:52:25 ON 03 SEP 2007

L1 STRUCTURE UPLOADED

L2 50 S L1 SSS SAM

L3 757409 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:53:00 ON 03 SEP 2007

FILE 'STNGUIDE' ENTERED AT 16:53:21 ON 03 SEP 2007

FILE 'REGISTRY' ENTERED AT 16:53:30 ON 03 SEP 2007

L4 1206 S SOLID

L5 111864 S L3 AND (PATENT)/DT

L6 0 S L3 AND (NUCLEOTIDE)

FILE 'HCAPLUS' ENTERED AT 16:54:58 ON 03 SEP 2007

L7 14183 S L5

FILE 'STNGUIDE' ENTERED AT 16:55:33 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 16:56:12 ON 03 SEP 2007

L8 117385 S SOLID PHASE

L9 197 S L7 AND L8

L10 757038 S NUCLEO?

L11 20 S L9 AND L10

L12 14 S L11 AND 1800<=PY<=2004

FILE 'STNGUIDE' ENTERED AT 16:57:51 ON 03 SEP 2007

FILE 'REGISTRY' ENTERED AT 16:58:52 ON 03 SEP 2007

L13 86865 S L3 AND (JOURNAL)/DT

FILE 'HCAPLUS' ENTERED AT 16:59:25 ON 03 SEP 2007

L14 26804 S L13

L15 834 S L14 AND L10

L16 35 S L8 AND L15

L17 28 S L16 AND 1800<=PY<=2004

FILE 'STNGUIDE' ENTERED AT 17:01:24 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 17:01:47 ON 03 SEP 2007

L18 36 S L17 OR L12

L19 787239 S GLASS

L20 1 S L19 AND L18

FILE 'STNGUIDE' ENTERED AT 17:02:19 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 17:02:27 ON 03 SEP 2007

L21 2211063 S TRITYL OR TRT OR SIL?

L22 2 S L21 AND L18

FILE 'STNGUIDE' ENTERED AT 17:02:55 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 17:03:50 ON 03 SEP 2007

E NGO NAM/AU 25

L23 37 S (E1 OR E2 OR E3 OR E4 OR E5 OR E6 OR E7 OR E8)

E JAQUINOD LAURENT/AU 25

L24 53 S (E2 OR E3)

E WANG HONG/AU 25

L25 2532 S (E3)

L26 88 S L23 OR L24
L27 5 S L26 AND L8
L28 0 S L27 AND (L7 OR L14)
L29 1 S L26 AND (L7 OR L14)

FILE 'STNGUIDE' ENTERED AT 17:06:46 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 17:06:58 ON 03 SEP 2007

E CATECHOL+ALL/CT

L30 453649 S (CATECHOL OR "CHEMICAL COMPOUNDS" OR "ORGANIC COMPOUNDS" OR "
L31 3442 S L30 AND L8
L32 484 S L31 AND L21
L33 2 S L31 AND L26
L34 377 S L32 AND 1800<=PY<=2004
L35 31 S L34 AND L19

FILE 'STNGUIDE' ENTERED AT 17:09:16 ON 03 SEP 2007

FILE 'HCAPLUS' ENTERED AT 17:29:14 ON 03 SEP 2007

E US20050182241/PN 25

L36 1 S E3

FILE 'STNGUIDE' ENTERED AT 17:30:02 ON 03 SEP 2007

FILE 'REGISTRY' ENTERED AT 17:30:49 ON 03 SEP 2007

L37 3 S 91-16-7 OR 120-80-9 OR 18156-74-6

FILE 'HCAPLUS' ENTERED AT 17:30:59 ON 03 SEP 2007

L38 25941 S L37
L39 745 S L38 AND (L7 OR L14)
L40 57 S L39 AND L21
L41 457 S L39 AND L30
L42 10 S L39 AND L19
L43 6 S L39 AND L8
L44 16 S L42 OR L43
L45 6 S L44 AND 1800<=PY<=2004

L12 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2007:202060 HCAPLUS
 DOCUMENT NUMBER: 146:274627
 TITLE: Reverse-turn mimetics for use as therapeutic and diagnostic agents
 INVENTOR(S): Moon, Sung Hwan; Chung, Jae Uk; Lee, Sung Chan; Eguchi, Masakatsu; Kahn, Michael; Jeong, Kwang Won; Nguyen, Cu; Lee, Soo Jin
 PATENT ASSIGNEE(S): Choongwae Pharma Corporation, S. Korea
 SOURCE: U.S. Pat. Appl. Publ., 223pp., Cont.-in-part of U.S. Ser. No. 826,972.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 6
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2007043052	A1	20070222	US 2005-108164	20050415
WO 2003031448	A1	20030417	WO 2002-KR1901	20021011 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CN 1872856	A	20061206	CN 2006-10093786	20021011
CN 1872857	A	20061206	CN 2006-10093787	20021011
US 2004072831	A1	20040415	US 2003-411877	20030409 <--
US 2007021431	A1	20070125	US 2004-803179	20040317
US 7232822	B2	20070619		
US 2007021425	A1	20070125	US 2004-826972	20040416
PRIORITY APPLN. INFO.:			US 2001-976470	B2 20011012
			US 2002-87443	B2 20020301
			WO 2002-KR1901	A 20021011
			US 2003-411877	B2 20030409
			US 2004-803179	A2 20040317
			US 2004-826972	A2 20040416
			CN 2002-822567	A3 20021011
OTHER SOURCE(S):		MARPAT 146:274627		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention discloses conformationally-constrained compds., e.g., I [Ra = (un)substituted phenyl; Rb = 5-7 membered monocyclic aryl; Rc = alkyl, alkoxy, perfluoroalkyl; X1, X2, X3 = independently H, OH, halo], that mimic the secondary structure of reverse-turn regions of biol. active peptides and proteins. The invention also discloses compds. of formula I-Y-R10 [Y = O, S, N, or a group selected from Ra, Rb, Rc, X1-X3; R10 = dimethylaminoalkylaminocarbonyloxy, hydroxyalkyl, glycosyl, etc.] that are capable of serving as substrates for a phosphatase or a carboxylase and are thereby converted to I. Such reverse-turn mimetic structures have utility over a wide range of fields, including use as diagnostic and therapeutic agents. Libraries containing the reverse-turn mimetic structures

of the invention are also disclosed and methods for screening them to identify biol. active members. The invention also relates to the use of such compds. for inhibiting or treating disorders modulated by Wnt-signaling pathway, such as cancer, especially colorectal cancer, restenosis associated with angioplasty, polycystic kidney disease, aberrant angiogenesis disease, rheumatoid arthritis disease, tuberous sclerosis complex, Alzheimer's disease, excess hair growth or loss, or ulcerative colitis. Thus, triazolopyrazinone derivative II was prepared using a bromoacetal resin and showed growth inhibition GI50 = 0.980 µg/mL against SW480-CWP cells.

IT 512856-58-5P 870887-94-8P

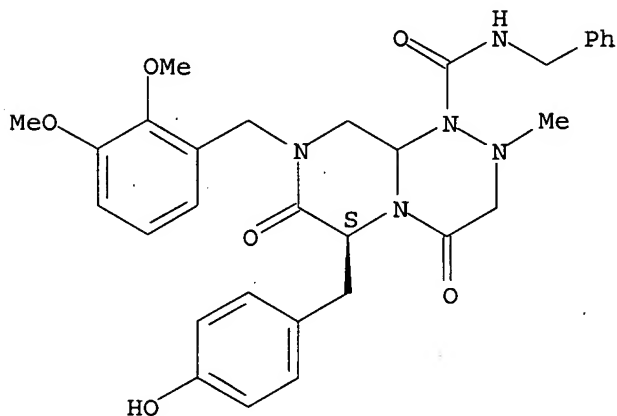
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of reverse-turn mimetics for use as therapeutic and diagnostic agents)

RN 512856-58-5 HCAPLUS

CN 2H-Pyrazino[2,1-c][1,2,4]triazine-1(6H)-carboxamide, 8-[(2,3-dimethoxyphenyl)methyl]hexahydro-6-[(4-hydroxyphenyl)methyl]-2-methyl-4,7-dioxo-N-(phenylmethyl)-, (6S)- (CA INDEX NAME)

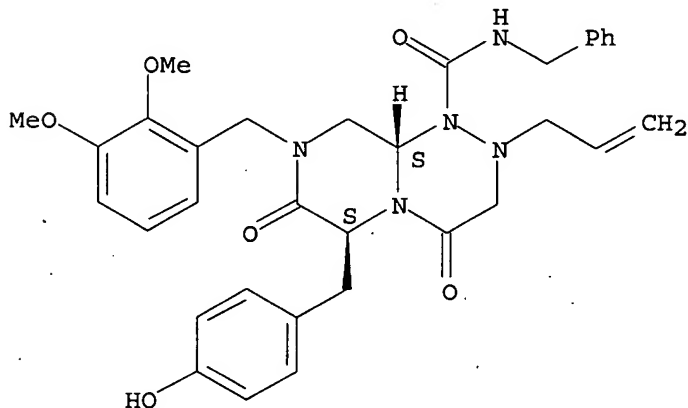
Absolute stereochemistry.



RN 870887-94-8 HCAPLUS

CN 2H-Pyrazino[2,1-c][1,2,4]triazine-1(6H)-carboxamide, 8-[(2,3-dimethoxyphenyl)methyl]hexahydro-6-[(4-hydroxyphenyl)methyl]-4,7-dioxo-N-(phenylmethyl)-2-(2-propen-1-yl)-, (6S,9aS)- (CA INDEX NAME)

Absolute stereochemistry.

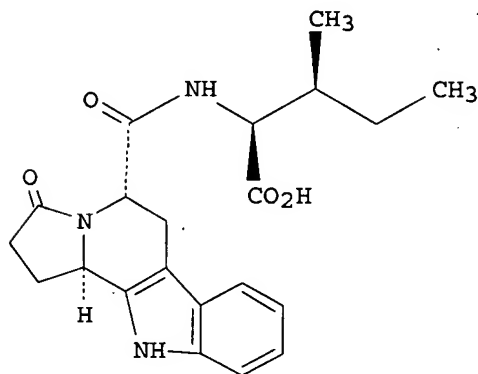


L12 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1156569 HCAPLUS
 DOCUMENT NUMBER: 142:74842
 TITLE: Synthesis of heterocyclic organic molecules through intramolecular formation of n-acyliminium ions using solid-phase synthesis techniques as combinatorial library components or for diagnostic use
 INVENTOR(S): Meldal, Morten; Nielsen, Thomas Eiland
 PATENT ASSIGNEE(S): Carlsberg A/S, Den.
 SOURCE: PCT Int. Appl., 111 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004113362	A2	20041229	WO 2004-DK454	20040625 <--
WO 2004113362	A3	20050210		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004249363	A1	20041229	AU 2004-249363	20040625 <--
CA 2533480	A1	20041229	CA 2004-2533480	20040625 <--
EP 1648921	A2	20060426	EP 2004-738951	20040625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2006252093	A1	20061109	US 2005-561803	20051222
IN 2006CN00319	A	20070706	IN 2006-CN319	20060125
PRIORITY APPLN. INFO.:			DK 2003-967	A 20030626
			DK 2004-820	A 20040525
			WO 2004-DK454	W 20040625

OTHER SOURCE(S): MARPAT 142:74842
 GI



I

AB The present invention relates to a method of preparing heterocyclic organic

comps., e.g. (I), involving intramol. formation of an N-acyliminium ion and a stereo-specific intramol. Pictet-Spengler reaction. These reactions were carried out using solid-phase peptide synthesis techniques. The invention furthermore discloses precursor mols., masked aldehyde building blocks (MABBs), useful for the method and methods of preparing these precursor mols. The invention also relates to heterocyclic organic comps. prepared by the methods, libraries of such heterocyclic organic compound and methods of preparing them, as well as to various uses of the heterocyclic organic comps (no data). Thus, resin-bound MABB-(substituted) (DL- or L-)Trp-L-Ile was prepared, and the MABB unmasked to form a reactive aldehyde, which participated in an intramol. Pictet Spengler cyclocondensation to give, in the case of L-Trp, I after resin cleavage. Title comps. and methods are claimed as useful for combinatorial chemical methods, as cell surface mol. association agents, e.g., for proteins, and for affinity chromatog. uses (no data).

IT 712351-20-7DP, resin-bound

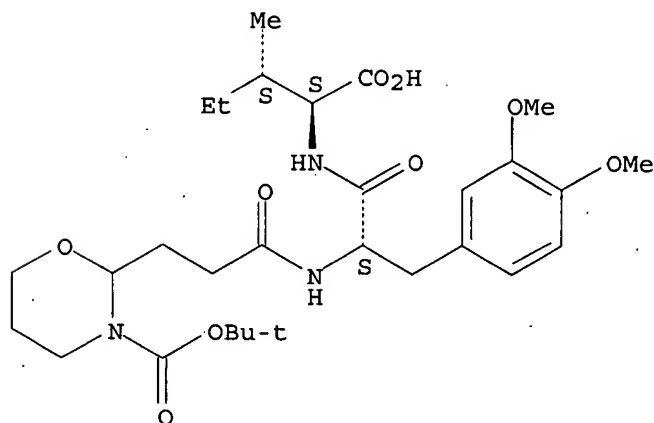
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and use of heterocyclic organic mols. through intramol. formation of n-acyliminium ions using solid-phase synthesis techniques as combinatorial library components or for diagnostic use)

RN 712351-20-7 HCAPLUS

CN L-Isoleucine, N-[3-[3-[(1,1-dimethylethoxy)carbonyl]tetrahydro-2H-1,3-oxazin-2-yl]-1-oxopropyl]-3-methoxy-O-methyl-L-tyrosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 712351-25-2P

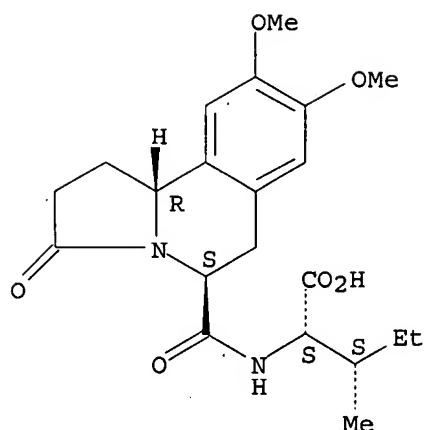
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and use of heterocyclic organic mols. through intramol. formation of n-acyliminium ions using solid-phase synthesis techniques as combinatorial library components or for diagnostic use)

RN 712351-25-2 HCAPLUS

CN L-Isoleucine, N-[[[(5S,10bR)-1,2,3,5,6,10b-hexahydro-8,9-dimethoxy-3-oxopyrrolo[2,1-a]isoquinolin-5-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1081989 HCAPLUS

DOCUMENT NUMBER: 142:54734

TITLE: Methods comprising T cell receptor and MHC antigen for high throughput screening of immunomodulators

INVENTOR(S): Rhode, Peter R.; Wittman, Vaughan; Weidanz, Jon A.; Burkhardt, Martin; Card, Kimberly F.; Tal, Rony; Acevedo, Jorge; Wong, Hing C.

PATENT ASSIGNEE(S): Sunol Molecular Corporation, USA

SOURCE: U.S. Pat. Appl. Publ., 95 pp., Cont.-in-part of U.S. Provisional Ser. No. 206,920.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

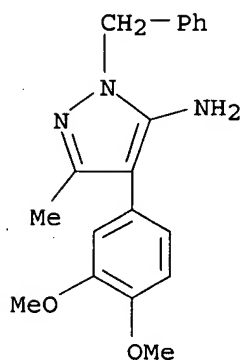
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004253632	A1	20041216	US 2001-859012	20010516 <--
PRIORITY APPLN. INFO.:			US 2000-206920P	P 20000525

AB Disclosed are methods for identifying compds. that modulate an immune complex that includes a T cell receptor (TCR) and a major histocompatibility complex (MHC) antigen. The invention has many useful applications including providing high throughput screening assays for detecting compns. that can modulate an immune response. These immune response modulators are useful for treating immune surveillance, autoimmune disease such as multiple sclerosis, infection and proliferative disease such as cancer.

IT 807628-19-9
 RL: ANT (Analyte); BSU (Biological study, unclassified); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
 (methods comprising T cell receptor and MHC antigen for high throughput screening of immunomodulators)

RN 807628-19-9 HCAPLUS

CN 1H-Pyrazol-5-amine, 4-(3,4-dimethoxyphenyl)-3-methyl-1-(phenylmethyl)-(9CI) (CA INDEX NAME)



L12 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:1080895 HCAPLUS

DOCUMENT NUMBER: 142:56321

TITLE: Preparation of N-tetrazolyl
benzo[b]thiophenecarboxamides as phosphoinositide-3-
kinase (PI3K) inhibitors for the treatment of cancer,
inflammatory and cardiovascular diseases

INVENTOR(S): Connolly, Mike; Gogliotti, Rocco Dean; Lee, Helen
Tsenwhei; Plummer, Mark Stephen; Sexton, Karen Elaine;
Visnick, Melean

PATENT ASSIGNEE(S): Warner-Lambert Company LLC, USA

SOURCE: PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

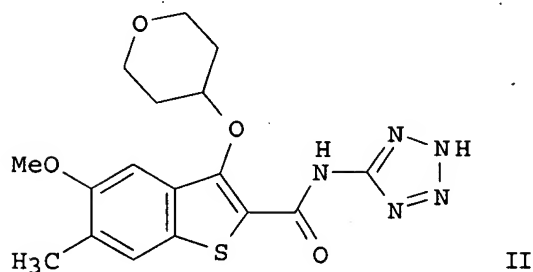
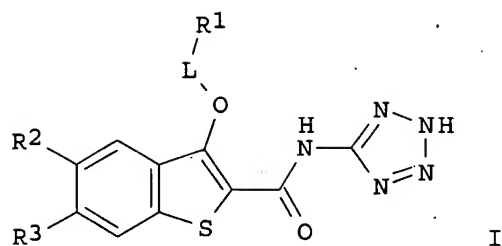
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004108713	A1	20041216	WO 2004-IB1783	20040524 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2527573	A1	20041216	CA 2004-2527573	20040524 <--
EP 1636210	A1	20060322	EP 2004-734574	20040524
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004010913	A	20060627	BR 2004-10913	20040524
JP 2006526606	T	20061124	JP 2006-508419	20040524
US 2005020630	A1	20050127	US 2004-860524	20040603
MX 2005PA13061	A	20060302	MX 2005-PA13061	20051202
PRIORITY APPLN. INFO.:			US 2003-476073P	P 20030605
			WO 2004-IB1783	W 20040524

OTHER SOURCE(S): MARPAT 142:56321

GI



AB Title compds. I [wherein R1 = (un)substituted cycloalk(en)yl or 4/5/6-membered heterocycloalkyl; R2, R3 = Me or OMe; L = absence or alkylene; with some limitations, and pharmaceutically acceptable salts thereof] were prepared as phosphoinositide-3-kinase (PI3K) inhibitors. For example, benzo[b]thiophenecarboxamide II was synthesized in several steps starting from 3-methoxy-4-methylbenzaldehyde. I were tested in several biol. assays, and showed inhibitory activity against PI3K with IC50 (μM) values of 0.003-2.550 (0.024 for II). Therefore, I and their pharmaceutical compns. are useful in the treatment of diseases and conditions, including inflammatory diseases, cardiovascular diseases, and cancers.

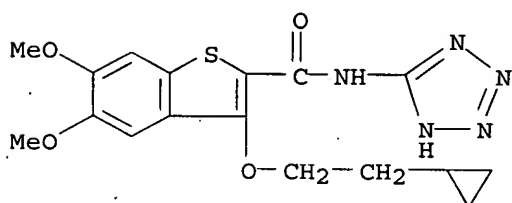
IT 809281-75-2P 809281-76-3P 809281-77-4P
 809281-78-5P 809281-79-6P 809281-80-9P
 809281-81-0P 809281-82-1P 809281-83-2P
 809281-84-3P 809281-85-4P 809281-86-5P
 809281-87-6P 809281-88-7P 809281-89-8P
 809281-90-1P 809281-91-2P 809281-95-6P
 809281-96-7P 809281-97-8P 809281-98-9P
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 809282-02-8P 809282-03-9P 809282-04-0P
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 809282-08-4P 810685-58-6P

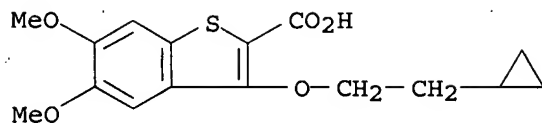
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(PI3K inhibitor; preparation of N-tetrazolyl benzo[b]thiophenecarboxamides as phosphoinositide-3-kinase (PI3K) inhibitors)

RN 809281-75-2 HCAPLUS

CN Benzo[b]thiophene-2-carboxamide, 3-(2-cyclopropylethoxy)-5,6-dimethoxy-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:707300 HCAPLUS

DOCUMENT NUMBER: 141:366181

TITLE: Solid phase synthesis of an extensively focused library of thiadiazole ethers

AUTHOR(S): Pernerstorfer, Josef; Brands, Michael; Schirok, Hartmut; Stelte-Ludwig, Beatrix; Woltering, Elisabeth

CORPORATE SOURCE: Bayer Health Care AG, Wuppertal, D-42096, Germany

SOURCE: Tetrahedron (2004), 60(39), 8627-8632

CODEN: TETRAB; ISSN: 0040-4020

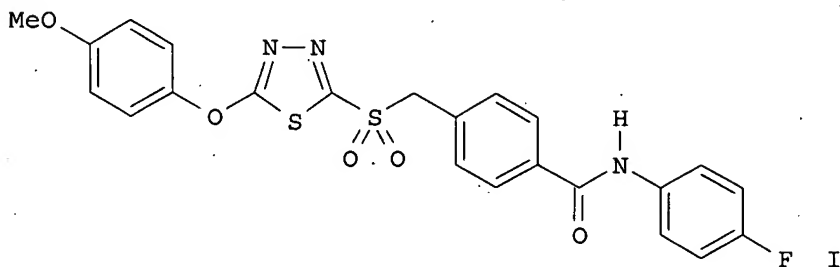
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:366181

GI



AB An approach to combine the advantages of random and of focused combinatorial libraries in pharmaceutical research, is described, with the example of a solid phase synthesis of 2,5-disubstituted thiadiazole ethers, e.g., I. Key steps of synthesis were the introduction of the heterocycle by selective, sequential nucleophilic double substitution of 2,5-bis(methylsulfonyl)-1,3,4-thiadiazole and the oxidation of the benzylsulfanyl-1,3,4-thiadiazole to the corresponding sulfone using MCPBA on solid phase.

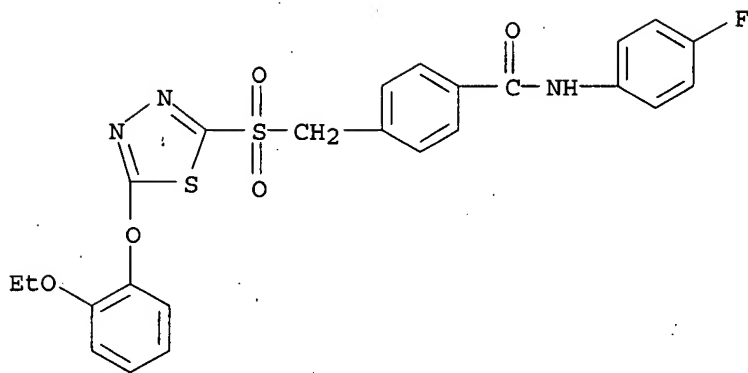
IT 500568-14-9P

RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation)

(combinatorial preparation, IL-8 inhibition, SAR of thiadiazole ethers via coupling of polymer-supported mercaptomethylbenzamides with bis(methylsulfonyl)thiadiazole followed by substitution with alcs. and oxidative resin cleavage)

RN 500568-14-9 HCAPLUS

CN Benzamide, 4-[[[5-(2-ethoxyphenoxy)-1,3,4-thiadiazol-2-yl]sulfonyl]methyl]-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:481966 HCAPLUS

DOCUMENT NUMBER: 141:190677

TITLE: Solid-Phase Synthesis of
1-Substituted Tetrahydroisoquinoline Derivatives
Employing BOC-Protected Tetrahydroisoquinoline
Carboxylic Acids

AUTHOR(S): Bunin, Barry A.; Dener, Jeffrey M.; Kelly, Daphne E.;
Paras, Nick A.; Tario, James D.; Tushup, Steven P.

CORPORATE SOURCE: ChemRx Division, Discovery Partners International,
South San Francisco, CA, 94080, USA

SOURCE: Journal of Combinatorial Chemistry (2004),
6(4), 487-496

CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:190677

AB Comps. containing the tetrahydroisoquinoline ring system were prepared using solid-supported ester derivs. on a nucleophile-sensitive resin, starting from the corresponding BOC-protected amino acids. The key heterocyclic intermediates were obtained from the Pictet-Spengler reaction between Et glyoxylate or Me 4-formylbenzoate and dopamine or 3-hydroxyphenethylamine. After the resulting amino esters were converted to the BOC derivs., the phenolic hydroxyl groups were alkylated with a series of alkyl halides to afford the corresponding ethers. Ester hydrolysis afforded the BOC-protected tetrahydroisoquinoline carboxylic acid scaffolds, which were then attached to (4-hydroxyphenyl)sulfide resin (Marshall linker) as the corresponding ester. The BOC group was removed under acidic conditions, and the resulting support-bound amine hydrochlorides were converted to the corresponding amides using a set of carboxylic acids. The support-bound amides were liberated with amines to produce the desired tetrahydroisoquinolinecarboxamides. Optimization of the resin loading conditions is described in addition to the identification of impurities observed during the development of the optimum conditions for solid-phase synthesis.

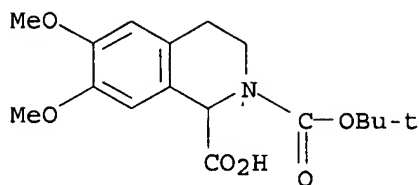
IT 738629-59-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase synthesis of N-acylated
tetrahydroisoquinolinecarboxamides via N-BOC protected
(hydroxyphenyl)sulfide resin-bound intermediates)

RN 738629-59-9 HCAPLUS

CN 1,2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-6,7-dimethoxy-,
2-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:355357 HCAPLUS

DOCUMENT NUMBER: 141:71467

TITLE: Solid-Phase Intramolecular
N-Acyliminium Pictet-Spengler Reactions as Crossroads
to Scaffold Diversity

AUTHOR(S): Nielsen, Thomas E.; Meldal, Morten

CORPORATE SOURCE: Department of Chemistry, Carlsberg Laboratory, Valby,
DK-2500, Den.

SOURCE: Journal of Organic Chemistry (2004), 69(11),
3765-3773

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:71467

AB A novel solid-phase intramol. Pictet-Spengler reaction is presented. The approach utilizes masked aldehyde building blocks protected as their N-Boc-1,3-oxazinones for the clean generation of solid-supported aldehydes. When exposed to simple acidic treatment, the aldehyde functionality is rapidly released and becomes susceptible to nucleophilic attack from an amide nitrogen of the peptide backbone, which results in the formation of a highly reactive cyclic N-acyliminium ion. Subsequently, a quant. and highly stereoselective Pictet-Spengler reaction takes place by attack of the indole from a neighboring tryptophan, thus appending two new N-fused rings to the indole moiety. Extension of this intramol. reaction to substituted indoles, and other reactive heterocycles, such as furane and thiophenes, provides a convenient and rapid access to a range of pharmacol. interesting tri- and tetracyclic scaffolds. Finally, the reaction products may conveniently be released from the solid support (PEGA) by cleavage of the base-labile linker (HMBA).

IT 712351-20-7P

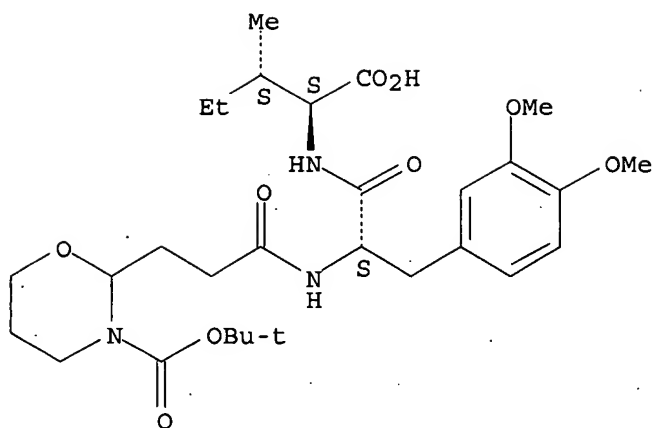
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fused (octahydro)indolizines from solid-phase intramol. Pictet-Spengler cyclocondensations of tryptophan peptides containing masked aldehydes as oxazinones)

RN 712351-20-7 HCAPLUS

CN L-Isoleucine, N-[3-[3-[(1,1-dimethylethoxy)carbonyl]tetrahydro-2H-1,3-oxazin-2-yl]-1-oxopropyl]-3-methoxy-O-methyl-L-tyrosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



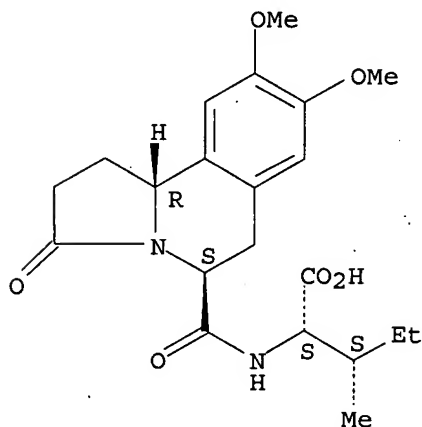
IT 712351-25-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of fused (octahydro)indolizines from solid-phase intramol. Pictet-Spengler cyclocondensations of tryptophan peptides containing masked aldehydes as oxazinones)

RN 712351-25-2 HCAPLUS

CN L-Isoleucine, N-[[[(5S,10bR)-1,2,3,5,6,10b-hexahydro-8,9-dimethoxy-3-oxopyrrolo[2,1-a]isoquinolin-5-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:252228 HCAPLUS

DOCUMENT NUMBER: 140:287266

TITLE: Preparation of dihydropyrancarboxamides as e.g. kinesin inhibitors for treatment of proliferative disorders.

INVENTOR(S): Schreiber, Stuart L.; Stavenger, Robert A.; Mitchison, Timothy J.; Maliga, Zoltan

PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA

SOURCE: U.S. Pat. Appl. Publ., 115 pp.

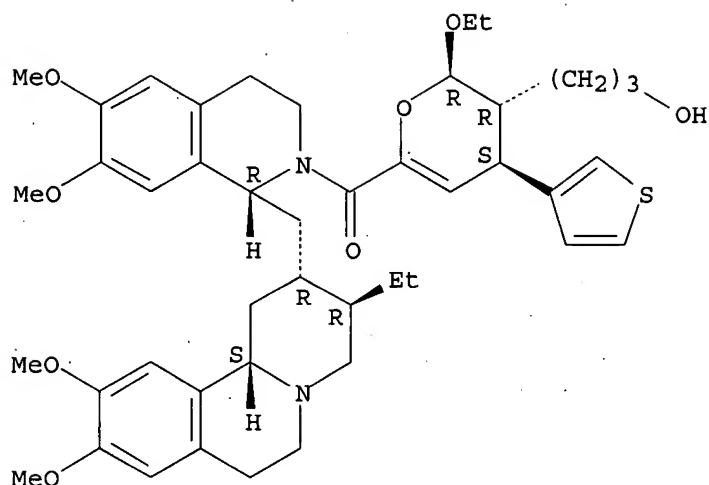
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:155114 HCAPLUS
 DOCUMENT NUMBER: 138:170465
 TITLE: Photo-cleavable protecting groups useful as linking groups in nucleoside synthesis, preferably in solid phase synthesis of oligonucleotides and polypeptides
 INVENTOR(S): Barone, Anthony; McGall, Glenn H.
 PATENT ASSIGNEE(S): Affymetrix, Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 51 pp., Cont.-in-part of U. S. Ser. No. 659,599.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003040618	A1	20030227	US 2001-950982	20010912 <--
US 2005101765	A1	20050512	US 2004-16380	20041217
PRIORITY APPLN. INFO.:			US 2000-659599	A2 20000911
			US 2001-950982	A1 20010912

OTHER SOURCE(S): MARPAT 138:170465

AB Novel compds. are provided which are useful as linking groups in chemical synthesis, preferably in the solid phase synthesis of oligonucleotides and polypeptides. These compds. are generally photo-labile and comprise protecting groups which can be removed by photolysis to unmask a reactive group.

IT 496956-64-0P

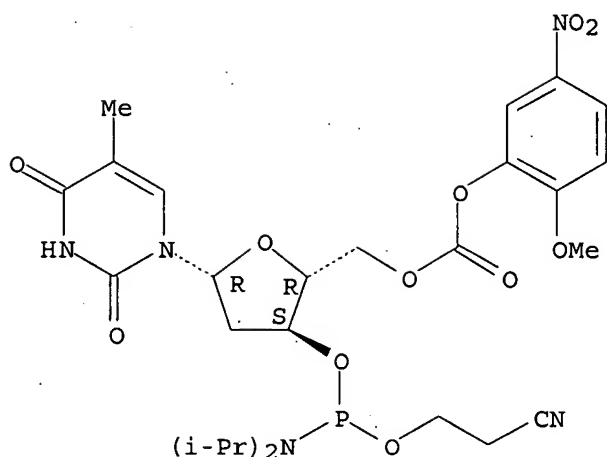
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(photo-cleavable protecting groups useful as linking groups in nucleoside synthesis, preferably in solid phase synthesis of oligonucleotides and polypeptides)

RN 496956-64-0 HCAPLUS

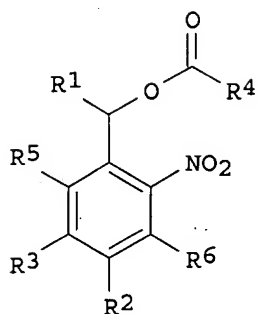
CN Thymidine, 3'-[2-cyanoethyl bis(1-methylethyl)phosphoramidite] 5'-(2-methoxy-5-nitrophenyl carbonate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:5916 HCAPLUS
 DOCUMENT NUMBER: 138:73466
 TITLE: Preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of nucleic acids
 INVENTOR(S): Serafinowski, Pawel Jerzy; Garland, Peter Bryan
 PATENT ASSIGNEE(S): The Institute of Cancer Research, UK
 SOURCE: PCT Int. Appl., 92 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000644	A1	20030103	WO 2002-GB2896	20020621 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW.				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002314335	A1	20030108	AU 2002-314335	20020621 <--
EP 1399412	A1	20040324	EP 2002-740905	20020621 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004242653	A1	20041202	US 2004-481707	20040716 <--
PRIORITY APPLN. INFO.:				
			GB 2001-15231	A 20010621
			GB 2001-22760	A 20010921
			WO 2002-GB2896	W 20020621
OTHER SOURCE(S): MARPAT 138:73466				
GI				



I

AB Nucleotides I wherein: R1 is selected from hydrogen, aryl or substituted aryl, aryloxy or substituted aryloxy, or an unsubstituted or substituted heterocyclic group; R2 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or a nitro group; R3 is selected from hydrogen, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or an unsubstituted or substituted heterocyclic group; R4 is an alkyl group substituted with one or more halogen substituents; R5 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, a nitro group or an unsubstituted or substituted heterocyclic group; and, R6 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, or amino or substituted amino, or an unsubstituted or substituted heterocyclic group, which are capable of generating acid on photolysis are disclosed, and the uses of these compds., especially for deprotecting the termini of nucleic acid mols. or peptides during synthesis of arrays. The compds. described herein may be employed in the detritylation of 5'-O-dimethoxytrityl (DMT) protected nucleotides by photolyzing the compds. to generate an acid capable of removing the DMT group allowing oligonucleotide arrays to be synthesized using readily available 5'-O-DMT-nucleoside-3'-O-phosphoramidite monomers conventionally used in solid phase nucleic acid synthesis. A method of avoiding the effects of stray light in projection lithog. techniques is also disclosed. Thus, α -phenyl-4,5-dimethoxy-2,6-dinitrobenzyltrichloroacetate was prepared and used in DNA synthesis.

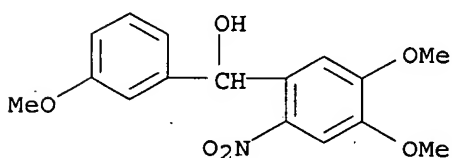
IT 479637-48-4P 479637-49-5P 479637-66-6P
479637-67-7P 479637-68-8P 479637-75-7P
479637-76-8P 479637-77-9P

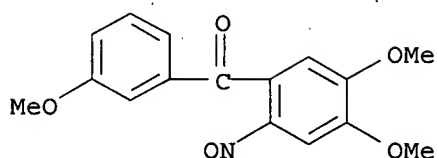
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of DNA)

RN 479637-48-4 HCAPLUS

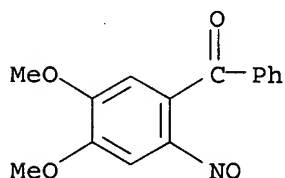
CN Benzenemethanol, 4,5-dimethoxy- α -(3-methoxyphenyl)-2-nitro- (9CI)
(CA INDEX NAME)





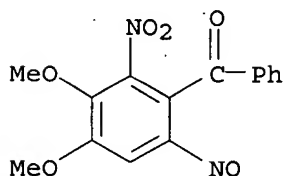
RN 479637-76-8 HCAPLUS

CN Methanone, (4,5-dimethoxy-2-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



RN 479637-77-9 HCAPLUS

CN Methanone, (3,4-dimethoxy-2-nitro-6-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:777948 HCAPLUS

DOCUMENT NUMBER: 137:311152

TITLE: Solid phase synthesis of cholesterol-linked and dye-labeled oligodeoxyribonucleotides

INVENTOR(S): Manoharan, Muthiah; Guzaev, Andrei

PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 111 pp.

CODEN: PIXXD2

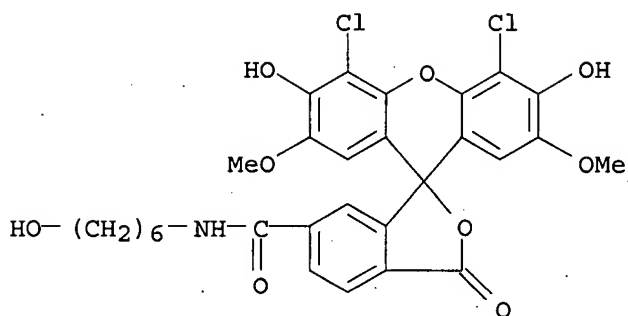
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079216	A1	20021010	WO 2002-US10178	20020329 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:314906 HCAPLUS

DOCUMENT NUMBER: 136:340491

TITLE: Preparation of sulfanilide derivatives as oxytocin and/or vasopressin receptor antagonists

INVENTOR(S): Quattropiani, Anna; Schwarz, Matthias; Jorand-Lebrun, Catherine; Church, Dennis; Scheer, Alexander

PATENT ASSIGNEE(S): Applied Research Systems Ars Holding N.V., Neth. Antilles

SOURCE: PCT Int. Appl., 187 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

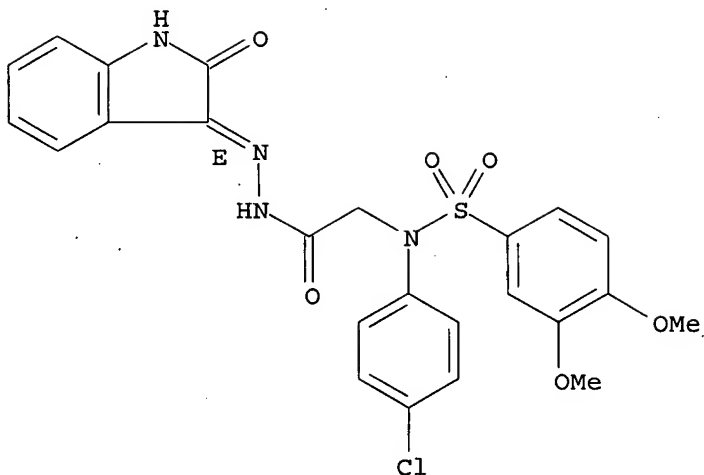
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032864	A1	20020425	WO 2001-EP11865	20011015 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2423933	A1	20020425	CA 2001-2423933	20011015 <--
AU 140192002	A	20020429	AU 2002-14019	20011015 <--
EP 1335901	A1	20030820	EP 2001-982432	20011015 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004511543	T	20040415	JP 2002-536048	20011015 <--
AU 2002214019	B2	20070125	AU 2002-214019	20011015
US 2004072816	A1	20040415	US 2003-399040	20030925 <--
AU 2007201854	A1	20070517	AU 2007-201854	20070426
PRIORITY APPLN. INFO.:				
			EP 2000-122588	A 20001017
			AU 2002-214019	A3 20011015
			WO 2001-EP11865	W 20011015

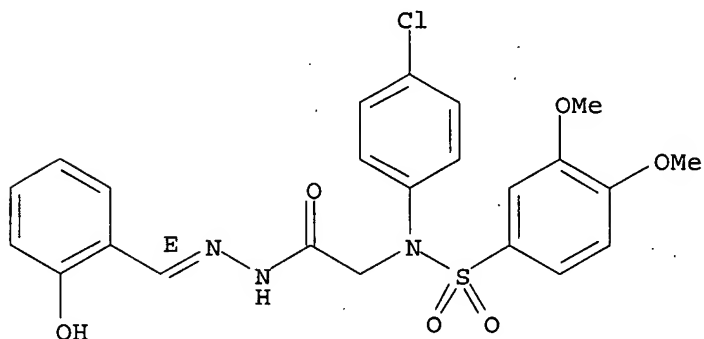
OTHER SOURCE(S): MARPAT 136:340491

GI



RN 415962-94-6 HCAPLUS
 CN Glycine, N-(4-chlorophenyl)-N-[(3,4-dimethoxyphenyl)sulfonyl]-,
 (2E)-[(2-hydroxyphenyl)methylene]hydrazide (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:293513 HCAPLUS
 DOCUMENT NUMBER: 136:306429
 TITLE: Linkers and their application for solid phase chemical synthesis
 INVENTOR(S): Weaver, George William; Smith, Adrian; Palmer, Derek Adeymi; French, Martin Thomas
 PATENT ASSIGNEE(S): Kalibrant Limited, UK
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030558	A2	20020418	WO 2001-GB4513	20011010 <--
WO 2002030558	A3	20020906		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
 PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
 US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

GB 2367818 A 20020417 GB 2000-24941 20001011 <--

AU 2001092140 A5 20020422 AU 2001-92140 20011010 <--

PRIORITY APPLN. INFO.:

GB 2000-24941 A 20001011

WO 2001-GB4513 W 20011010

AB The invention concerns dockable linkers for solid phase synthesis. These linkers would allow reactions to be conducted in homogeneous solution but still allow easy isolation and purification of reaction products at each step of a synthetic route. The process would also allow easy anal. of all intermediates generated.

IT 409332-82-7P

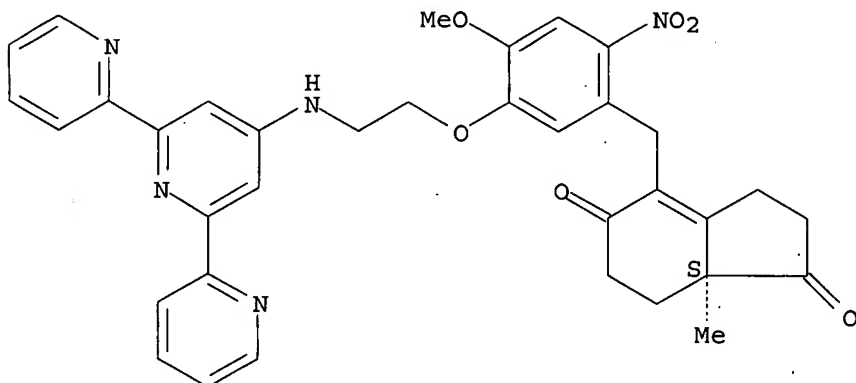
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(linkers and application for solid phase chemical synthesis)

RN 409332-82-7 HCAPLUS

CN 1H-Indene-1,5(6H)-dione, 2,3,7,7a-tetrahydro-4-[[4-methoxy-2-nitro-5-[2-([2,2':6',2''-terpyridin]-4'-ylamino)ethoxy]phenyl)methyl]-7a-methyl-, (7aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:240713 HCAPLUS

DOCUMENT NUMBER: 136:294650

TITLE: Preparation of substituted phenylacetamides and benzamides as agonists for Liver X receptors (LXR)

INVENTOR(S): Collins, Jon Loren; Fivush, Adam M.; Maloney, Patrick Reed; Stewart, Eugene L.; Willson, Timothy Mark

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 118 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

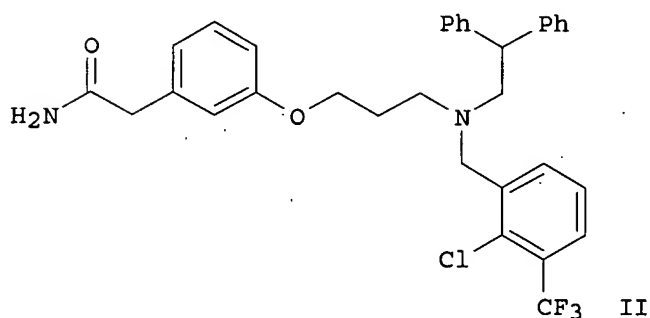
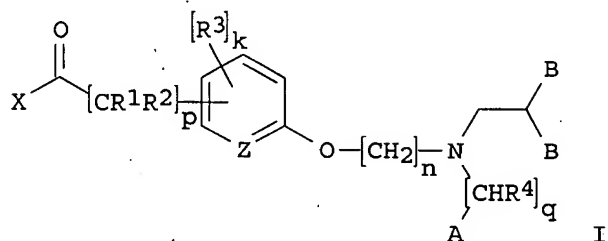
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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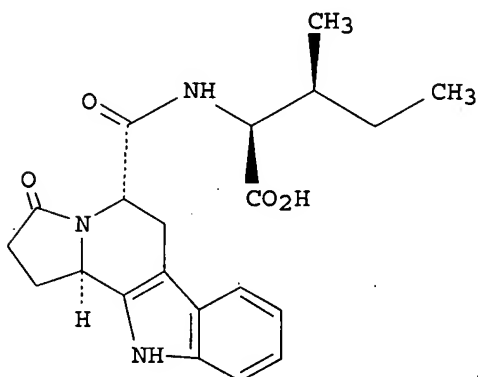
WO 2002024632 A2 20020328 WO 2001-US27622 20010906 <--
 WO 2002024632 A3 20020711
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 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
 PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
 US, UZ, VN, YU, ZA, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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 AU 2002011216 A5 20020402 AU 2002-11216 20010906 <--
 EP 1318976 A2 20030618 EP 2001-979230 20010906 <--
 EP 1318976 B1 20041124
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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 JP 2004509161 T 20040325 JP 2002-528647 20010906 <--
 AT 283253 T 20041215 AT 2001-979230 20010906 <--
 ES 2233700 T3 20050616 ES 2001-1979230 20010906
 US 2004072868 A1 20040415 US 2003-380932 20030318 <--
 US 2005282908 A1 20051222 US 2005-154852 20050616
 PRIORITY APPLN. INFO.: US 2000-233144P P 20000918
 WO 2001-US27622 W 20010906
 US 2003-380932 A1 20030318
 OTHER SOURCE(S): MARPAT 136:294650
 GI



AB The title compds. [I; X = OH, NH₂; p = 0-6; R₁, R₂ = H, alkyl, alkoxy, thioalkyl; Z = CH, N; when Z = CH, k = 0-4; when Z = N, k = 0-3; R₃ = halo, OH, alkyl, etc.; n = 2-8; q = 0-1; R₄ = H, alkyl, alkenyl, alkenyloxy; A = cycloalkyl, aryl, 4-8 membered heterocycle, 5-6 membered heteroaryl; B = cycloalkyl, aryl] and their pharmaceutically acceptable salts, useful for the prevention or treatment of an LXR mediated disease and condition such as cardiovascular disease and atherosclerosis (no biol. data given), were prepared E.g., a solid phase

SOURCE: PCT Int. Appl., 111 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

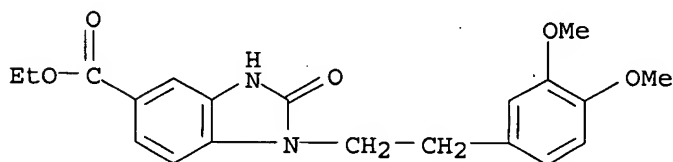
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004113362	A2	20041229	WO 2004-DK454	20040625 <--
WO 2004113362	A3	20050210		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004249363	A1	20041229	AU 2004-249363	20040625 <--
CA 2533480	A1	20041229	CA 2004-2533480	20040625 <--
EP 1648921	A2	20060426	EP 2004-738951	20040625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2006252093	A1	20061109	US 2005-561803	20051222
IN 2006CN00319	A	20070706	IN 2006-CN319	20060125
PRIORITY APPLN. INFO.:				
			DK 2003-967	A 20030626
			DK 2004-820	A 20040525
			WO 2004-DK454	W 20040625
OTHER SOURCE(S): MARPAT 142:74842				
GI				



I

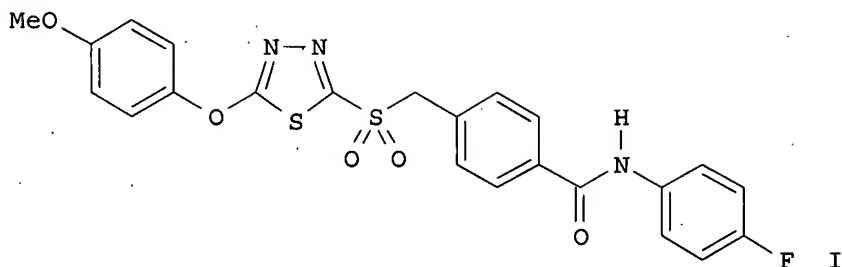
AB The present invention relates to a method of preparing heterocyclic organic compds., e.g. (I), involving intramol. formation of an N-acyliminium ion and a stereo-specific intramol. Pictet-Spengler reaction. These reactions were carried out using solid-phase peptide synthesis techniques. The invention furthermore discloses precursor mols., masked aldehyde building blocks (MABBs), useful for the method and methods of preparing these precursor mols. The invention also relates to heterocyclic organic compds. prepared by the methods, libraries of such heterocyclic organic compound and methods of preparing them, as well as to various uses of the heterocyclic organic compds (no data). Thus, resin-bound MABB-(substituted) (DL- or L-)Trp-L-Ile was prepared, and the MABB unmasked

L17 ANSWER 2 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:742166 HCAPLUS
DOCUMENT NUMBER: 141:395479
TITLE: Traceless Solid-Phase Synthesis of
Substituted Benzimidazolones
AUTHOR(S): Wang, Chih-Chung; Li, Wen-Ren
CORPORATE SOURCE: Department of Chemistry, National Central University,
Chung-Li, 32054, Taiwan
SOURCE: Journal of Combinatorial Chemistry (2004),
6(6), 899-902
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:395479
AB A new approach to substituted benzimidazolones is described. The key step
of the sequence involved the introduction of one of the nitrogens by
nucleophilic addition of a carbamate to an o-fluoronitrobenzene.
Spontaneous cyclization and detachment of the benzimidazolones from the
resin occurred in high yields under reductive conditions on solid
supports. To further expand the scale and incorporate a third element of
diversity into the library of target mols., the benzimidazolones were
treated with NaH and various alkyl halides in DMF to afford fully
functionalized benzimidazolones.
IT 785805-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(traceless solid-phase synthesis of substituted
benzimidazolones)
RN 785805-53-0 HCAPLUS
CN 1H-Benzimidazole-5-carboxylic acid, 1-[2-(3,4-dimethoxyphenyl)ethyl]-2,3-
dihydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:707300 HCAPLUS
DOCUMENT NUMBER: 141:366181
TITLE: Solid phase synthesis of an
extensively focused library of thiadiazole ethers
AUTHOR(S): Pernerstorfer, Josef; Brands, Michael; Schirok,
Hartmut; Stelte-Ludwig, Beatrix; Woltering, Elisabeth
CORPORATE SOURCE: Bayer Health Care AG, Wuppertal, D-42096, Germany
SOURCE: Tetrahedron (2004), 60(39), 8627-8632
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:366181
GI



AB An approach to combine the advantages of random and of focused combinatorial libraries in pharmaceutical research, is described, with the example of a solid phase synthesis of 2,5-disubstituted thiadiazole ethers, e.g., I. Key steps of synthesis were the introduction of the heterocycle by selective, sequential nucleophilic double substitution of 2,5-bis(methylsulfonyl)-1,3,4-thiadiazole and the oxidation of the benzylsulfanyl-1,3,4-thiadiazole to the corresponding sulfone using MCPBA on solid phase.

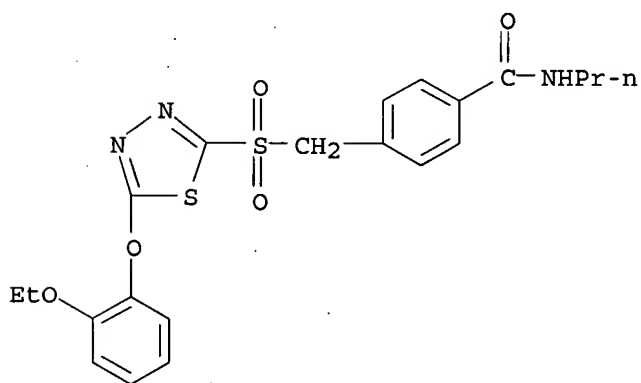
IT 777856-00-5P 777856-03-8P 777856-18-5P
 777856-20-9P 777856-21-0P 777856-23-2P
 777856-25-4P 777856-28-7P 777856-30-1P
 777856-31-2P 777856-33-4P 777856-35-6P
 777856-38-9P 777856-40-3P 777856-41-4P
 777856-43-6P 777856-45-8P 777856-48-1P
 777856-50-5P 777856-51-6P 777856-53-8P
 777856-55-0P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(combinatorial preparation of thiadiazole ethers via coupling of polymer-supported mercaptomethylbenzamides with bis(methylsulfonyl)thiadiazole followed by substitution with alcs. and oxidative resin cleavage)

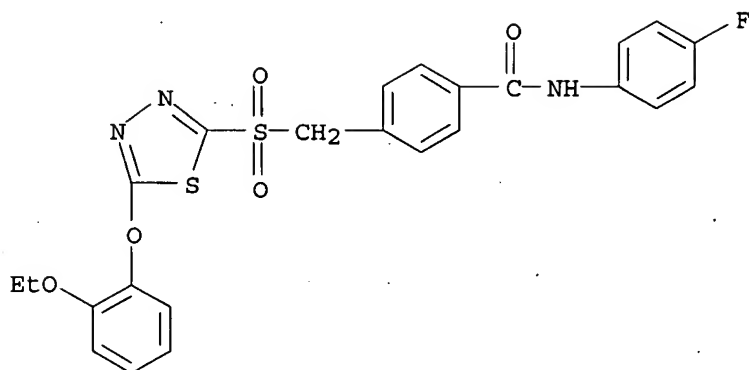
RN 777856-00-5 HCAPLUS

CN Benzamide, 4-[[[5-(2-ethoxyphenoxy)-1,3,4-thiadiazol-2-yl]sulfonyl]methyl]-N-propyl- (9CI) (CA INDEX NAME)



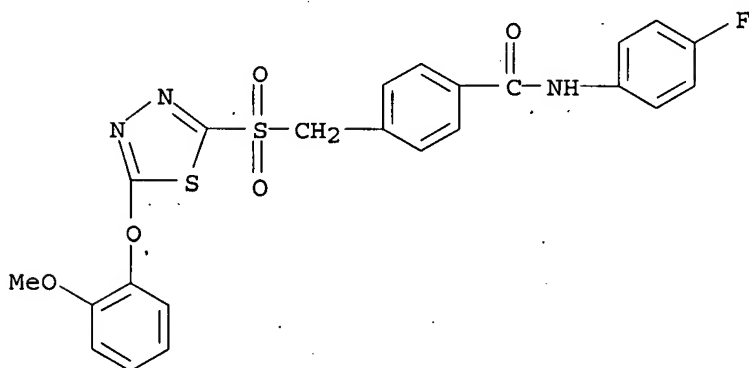
RN 777856-03-8 HCAPLUS

CN Benzamide, 4-[[[5-(2-methoxyphenoxy)-1,3,4-thiadiazol-2-yl]sulfonyl]methyl]-N-propyl- (9CI) (CA INDEX NAME)



RN 777855-82-0 HCAPLUS

CN Benzamide, N-(4-fluorophenyl)-4-[[[5-(2-methoxyphenoxy)-1,3,4-thiadiazol-2-yl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:707297 HCAPLUS

DOCUMENT NUMBER: 141:366096

TITLE: Solid-phase synthesis of isoindolinones and naturally-occurring benzobutyrolactones (phthalides) using a cyclative-cleavage approach

AUTHOR(S): Knepper, Kerstin; Ziegert, Robert E.; Brase, Stefan

CORPORATE SOURCE: Kekule-Institut für Organische Chemie Biochemie, Rheinischen Friedrich-Wilhelms-Universität Bonn, Bonn, D-53121, Germany

SOURCE: Tetrahedron (2004), 60(39), 8591-8603

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

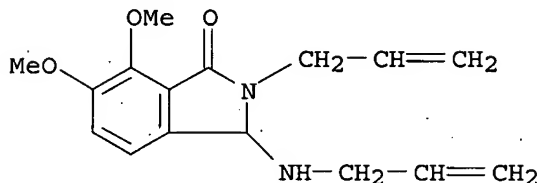
LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:366096

AB Starting from Merrifield resin, 2-formylbenzoic acids were immobilized on solid supports. Reactions between immobilized 2-formylbenzoic acids and different organometallic reagents (Grignard reagents, zinc reagents, allyl silanes via Sakurai type reactions) furnished secondary alcs. which cyclized depending on the metal counter ion and reaction conditions, forming benzoannelated lactones. Asym. synthesis was possible on the resin using chiral [2.2]paracyclophane ligands. While the reaction of immobilized ortho-carboxy benzaldehydes with primary amines at elevated

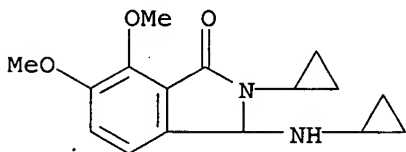
RN 779328-85-7 HCAPLUS

CN 1H-Isoindol-1-one, 2,3-dihydro-6,7-dimethoxy-2-(2-propenyl)-3-(2-propenylamino)- (9CI) (CA INDEX NAME)



RN 779328-86-8 HCAPLUS

CN 1H-Isoindol-1-one, 2-cyclopropyl-3-(cyclopropylamino)-2,3-dihydro-6,7-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:635045 HCAPLUS

DOCUMENT NUMBER: 141:314242

TITLE: A solid-phase approach to fluorobenzimidazoles and fluoro-2-hydroxyquinoxalines using 'one-bead-two-compound' method

AUTHOR(S): Ji, Ya-Fei; Pan, Xian-Dao; Wei, Xian-Yong

CORPORATE SOURCE: Department of Pharmacy Engineering, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China

SOURCE: Synlett (2004), (9), 1607-1609

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:314242

AB A solid-phase approach to fluorobenzimidazoles and fluoro-2-hydroxyquinoxalines has been achieved by a new one-bead-two-compound strategy. The precursor, 6-nitro-2,3,4,5-tetrafluorobenzoic acid, was tagged to Rink amide MBHA resin via an α -amino acid linker. The first nucleophilic substitution generated two regioisomers in which the second active fluorine atom underwent a subsequent nucleophilic substitution with a primary amine. The reduction of the aryl nitro groups with $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}/\text{NMM}$ and the formation of a five-membered ring with aldehydes afforded polymer-supported products. The fluorobenzimidazoles were directly furnished by cleavage using TFA, while the stable six-membered ring in the 2-hydroxyquinoxalines was produced by concomitant intramolecular cyclization and thermal dehydrogenation. In addition to introduction of fluorine into the heterocycles, two scaffolds could be simultaneously synthesized with this method.

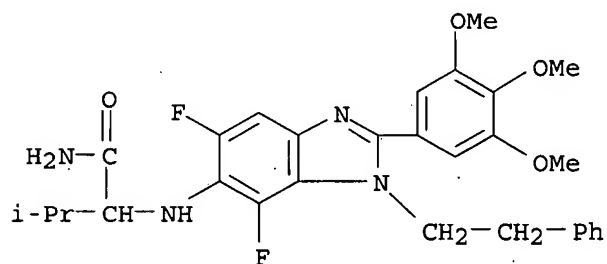
IT 765923-85-1P 765923-89-5P

RL: SPN (Synthetic preparation); PREP. (Preparation)

(a solid-phase approach to fluorobenzimidazoles and
fluoro-2-hydroxyquinoxalines using a one-bead-two-compound method)

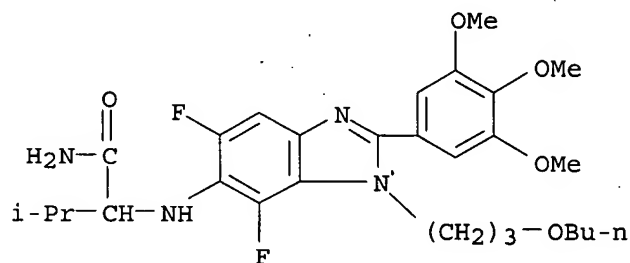
RN 765923-85-1 HCAPLUS

CN Butanamide, 2-[[5,7-difluoro-1-(2-phenylethyl)-2-(3,4,5-trimethoxyphenyl)-1H-benzimidazol-6-yl]amino]-3-methyl- (9CI) (CA INDEX NAME)



RN 765923-89-5 HCAPLUS

CN Butanamide, 2-[[1-(3-butoxypropyl)-5,7-difluoro-2-(3,4,5-trimethoxyphenyl)-1H-benzimidazol-6-yl]amino]-3-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l17 ibib abs hitstr 6-14

L17 ANSWER 6 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:607059 HCAPLUS

DOCUMENT NUMBER: 141:295796

TITLE: Titanium Reagents for the Synthesis of 2-Substituted Benzo[b]thiophenes on the Solid Phase

AUTHOR(S): Roberts, Christine F.; Hartley, Richard C.

CORPORATE SOURCE: Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK

SOURCE: Journal of Organic Chemistry (2004), 69(18), 6145-6148

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:295796

AB Titanium(IV) benzylidenes (Schrock carbenes) bearing a masked sulfur nucleophile in the ortho position were generated from thioacetals with use of low-valent titanocene complex $\text{Cp}_2\text{Ti}[\text{P}(\text{OEt})_3]_2$ and alkylidenated Merrifield resin-bound esters to give enol ethers. Treatment of the resin-bound enol ethers with a 5: 5:90 mixture of TFA, TFAA, and dichloromethane led to cleavage from resin, removal of the tert-butyldimethylsilyl (TBDMS) protecting group, and concomitant

OTHER SOURCE(S): CASREACT 142:155900
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Guanine-derived small mols. play important roles in many aspects of cellular function. Proteins that bind guanine and its derivs. control a wide variety of cellular processes, and compds. that disrupt this binding would be valuable research tools as well as potential pharmaceuticals. A split-pool library of 270 6-substituted-2-amino-4(3H)-quinazolinones (I) (R1 = residue of thiol, phenol, or primary alcs.; R2 = aryl or alkyl; e.g. R1 = 3,4-dimethylphenyl, R2 = 3,4,5-trimethoxyphenyl, benzyl; R1 = isobutylthio, R2 = 3-acetylphenyl; R1 = cyclohexylthio, R2 = 4-chlorophenyl) was prepared by aza-Wittig-mediated solid-phase synthesis which involves (1) nucleophilic aromatic substitution of a resin-bound 5-fluoro-2-nitrobenzamide with a variety of thiols, phenols, and primary alcs., (2) generation of a resin-bound iminophosphorane (II) (P = resin) by treatment with Ph₃P/Cl₃CCl₃/imidazole (3 h, 4°), (3) aza-Wittig reaction of the iminophosphoranes with one of 15 isocyanates (R₂-NCO) to yield a carbodiimide (III) (P = resin) followed by intermol. O-attack instead of the desired N attack to the carbodiimide to yield an 4-imino-4H-3,1-benzoxazine (IV), and (4) DBU-mediated isomerization to the desired 2-amino-4(3H)-quinazolinone (V) (P = resin) followed by resin cleavage. The compds. I were cell-permeable guanine-mimetics and screened for (a) the effect on the cytoskeleton and cell cycle progression by incubating the compds. with BS-C-1-(monkey) cells for 6 h, followed by fixing and staining for actin, DNA, and microtubules and (b) disruption of cellular trafficking. For example, I (R1 = isobutylthio, R2 = 3-acetylphenyl) disrupted both the actin and microtubule cytoskeleton, but did not arrest cells in mitosis.

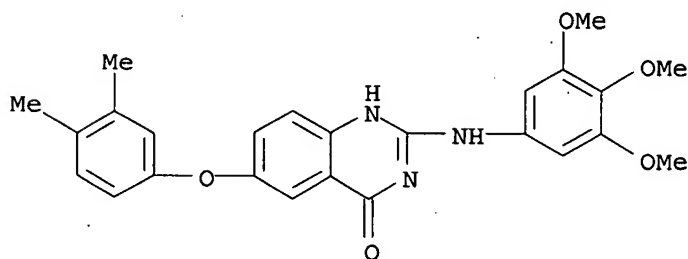
IT 828261-86-5P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)

(solid-phase synthesis and phenotypic screening of
guanine-mimetic library via aza-Wittig reaction of iminophosphoranes
with isocyanates and DBU-mediated isomerization iminobenzoxazines)

RN 828261-86-5 HCAPLUS

CN 4(1H)-Quinazolinone, 6-(3,4-dimethylphenoxy)-2-[(3,4,5-trimethoxyphenyl)amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 8 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:481966 HCAPLUS

DOCUMENT NUMBER: 141:190677

TITLE: Solid-Phase Synthesis of

1-Substituted Tetrahydroisoquinoline Derivatives
Employing BOC-Protected Tetrahydroisoquinoline
Carboxylic Acids

AUTHOR(S): Bunin, Barry A.; Dener, Jeffrey M.; Kelly, Daphne E.;
Paras, Nick A.; Tario, James D.; Tushup, Steven P.
CORPORATE SOURCE: ChemRx Division, Discovery Partners International,
South San Francisco, CA, 94080, USA
SOURCE: Journal of Combinatorial Chemistry (2004),
6(4), 487-496
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:190677

AB Compds. containing the tetrahydroisoquinoline ring system were prepared using solid-supported ester derivs. on a nucleophile-sensitive resin, starting from the corresponding BOC-protected amino acids. The key heterocyclic intermediates were obtained from the Pictet-Spengler reaction between Et glyoxylate or Me 4-formylbenzoate and dopamine or 3-hydroxyphenethylamine. After the resulting amino esters were converted to the BOC derivs., the phenolic hydroxyl groups were alkylated with a series of alkyl halides to afford the corresponding ethers. Ester hydrolysis afforded the BOC-protected tetrahydroisoquinoline carboxylic acid scaffolds, which were then attached to (4-hydroxyphenyl)sulfide resin (Marshall linker) as the corresponding ester. The BOC group was removed under acidic conditions, and the resulting support-bound amine hydrochlorides were converted to the corresponding amides using a set of carboxylic acids. The support-bound amides were liberated with amines to produce the desired tetrahydroisoquinolinecarboxamides. Optimization of the resin loading conditions is described in addition to the identification of impurities observed during the development of the optimum conditions for solid-phase synthesis.

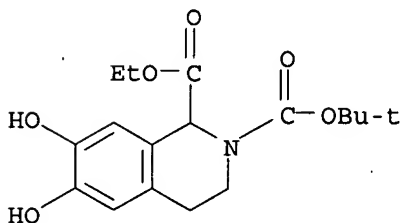
IT 738629-56-6P 738629-57-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(O-alkylation of hydroxytetrahydroisoquinoline derivative in solid phase synthesis of N-acylated tetrahydroisoquinolinecarboxamides via N-BOC protected (hydroxyphenyl)sulfide resin-bound intermediates)

RN 738629-56-6 HCAPLUS

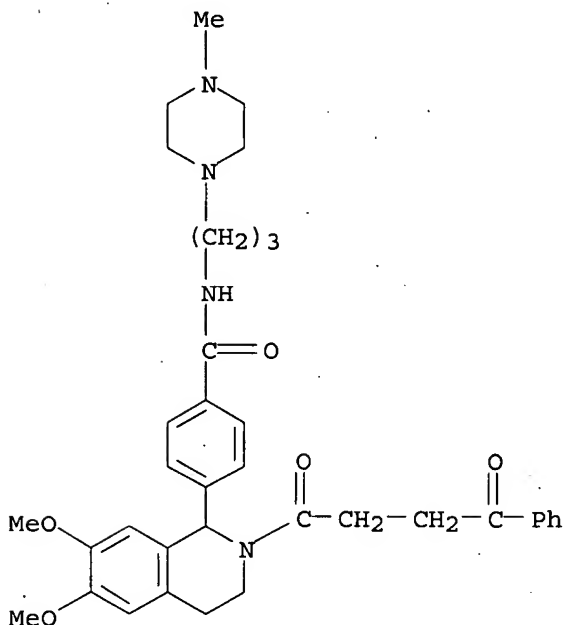
CN 1,2(1H)-Isoquinolinedicarboxylic acid, 3,4-dihydro-6,7-dihydroxy-, 2-(1,1-dimethylethyl) 1-ethyl ester (9CI) (CA INDEX NAME)



RN 738629-57-7 HCAPLUS

CN 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-6,7-dihydroxy-1-[4-(methoxycarbonyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 738629-66-8 HCAPLUS
 CN Benzamide, 4-[2-(1,4-dioxo-4-phenylbutyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinoliny]-N-[3-(4-methyl-1-piperazinyl)propyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:355357 HCAPLUS

DOCUMENT NUMBER: 141:71467

TITLE: Solid-Phase Intramolecular
 N-Acyliminium Pictet-Spengler Reactions as Crossroads
 to Scaffold Diversity

AUTHOR(S): Nielsen, Thomas E.; Meldal, Morten

CORPORATE SOURCE: Department of Chemistry, Carlsberg Laboratory, Valby,
 DK-2500, Den.

SOURCE: Journal of Organic Chemistry (2004), 69(11),
 3765-3773

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:71467

AB A novel solid-phase intramol. Pictet-Spengler reaction is presented. The approach utilizes masked aldehyde building blocks protected as their N-Boc-1,3-oxazinones for the clean generation of solid-supported aldehydes. When exposed to simple acidic treatment, the aldehyde functionality is rapidly released and becomes susceptible to nucleophilic attack from an amide nitrogen of the peptide backbone, which results in the formation of a highly reactive cyclic N-acyliminium ion. Subsequently, a quant. and highly stereoselective Pictet-Spengler reaction takes place by attack of the indole from a neighboring tryptophan, thus appending two new N-fused rings to the indole moiety. Extension of this intramol. reaction to substituted indoles, and other reactive heterocycles, such as furane and thiophenes, provides a convenient and rapid access to a range of pharmacol. interesting tri- and tetracyclic scaffolds. Finally, the reaction products may conveniently be

released from the solid support (PEGA) by cleavage of the base-labile linker (HMBA).

IT 712351-20-7P

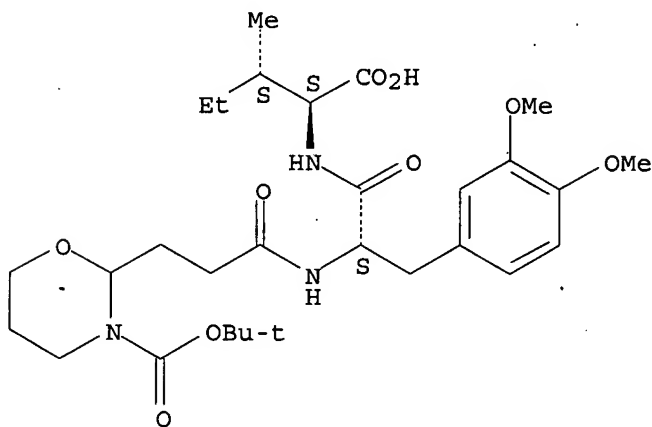
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fused (octahydro)indolizines from solid-phase intramol. Pictet-Spengler cyclocondensations of tryptophan peptides containing masked aldehydes as oxazinones)

RN 712351-20-7 HCAPLUS

CN L-Isoleucine, N-[3-[3-[(1,1-dimethylethoxy)carbonyl]tetrahydro-2H-1,3-oxazin-2-yl]-1-oxopropyl]-3-methoxy-O-methyl-L-tyrosyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



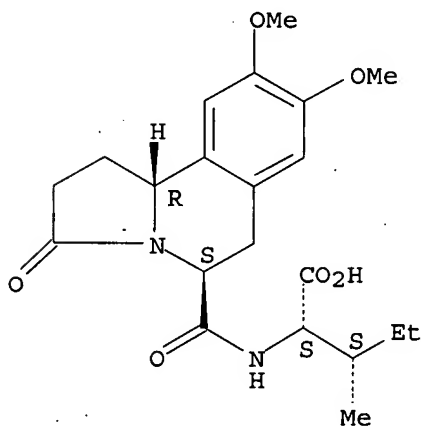
IT 712351-25-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fused (octahydro)indolizines from solid-phase intramol. Pictet-Spengler cyclocondensations of tryptophan peptides containing masked aldehydes as oxazinones)

RN 712351-25-2 HCAPLUS

CN L-Isoleucine, N-[[[(5S,10bR)-1,2,3,5,6,10b-hexahydro-8,9-dimethoxy-3-oxopyrrolo[2,1-a]isoquinolin-5-yl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

73

THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:236703 HCAPLUS

DOCUMENT NUMBER: 140:423636

TITLE: Solid-Phase Synthesis of
2,4-Diaminopyrimidines via Lewis Acid-Mediated
Aromatic Nucleophilic SubstitutionAUTHOR(S): Arvanitis, Elena A.; Chadha, Naresh; Pottorf, Richard
S.; Player, Mark R.CORPORATE SOURCE: 3-Dimensional Pharmaceuticals Inc., Cranbury, NJ,
08512, USASOURCE: Journal of Combinatorial Chemistry (2004),
6(3), 414-419

CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:423636

AB Primary amines were immobilized on (4-formyl-3,5-dimethoxyphenoxy)methylpolystyrene resin via reductive amination. Attachment of two different 4-chloro-2-methylthiopyrimidines, followed by sulfide oxidation, led to the sulfone intermediates. Aromatic nucleophilic substitution with various anilines or heteroarom. amines in the presence of trimethylaluminum afforded the desired 2,4-diaminopyrimidines after acidic cleavage from the resin. The synthetic methodol. described herein was validated with the synthesis of a small 162-member library.

IT 691403-24-4P 691403-26-6P 691403-28-8P

691403-30-2P 691403-32-4P 691403-34-6P

691403-36-8P 691403-38-0P 691403-41-5P

691405-34-2P 691405-37-5P 691405-39-7P

691405-41-1P 691405-43-3P 691405-45-5P

691405-48-8P 691405-50-2P 691405-52-4P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP
(Preparation)

(solid-phase combinatorial synthesis of

2,4-diaminopyrimidines via Lewis acid-mediated aromatic
nucleophilic substitution)

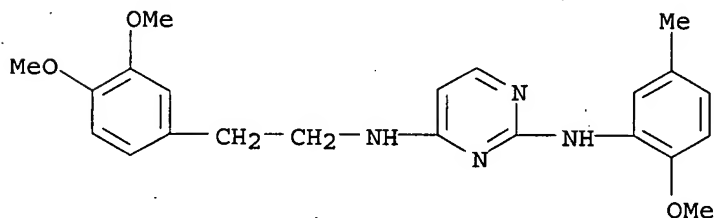
RN 691403-24-4 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-(2-methoxy-5-methylphenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691403-23-3

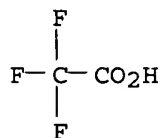
CMF C22 H26 N4 O3



CM 2

CRN 76-05-1

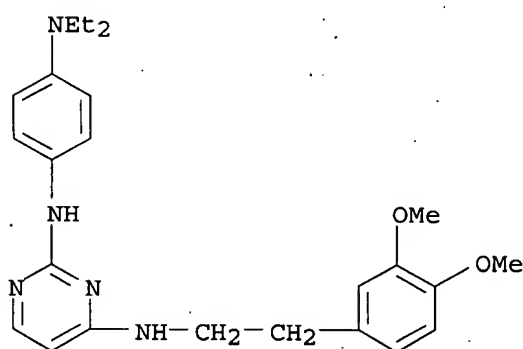
CMF C2 H F3 O2



RN 691403-26-6 HCAPLUS
 CN 2,4-Pyrimidinediamine, N2-[4-(diethylamino)phenyl]-N4-[2-(3,4-dimethoxyphenyl)ethyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

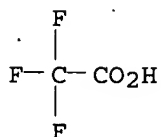
CM 1

CRN 691403-25-5
 CMF C24 H31 N5 O2



CM 2

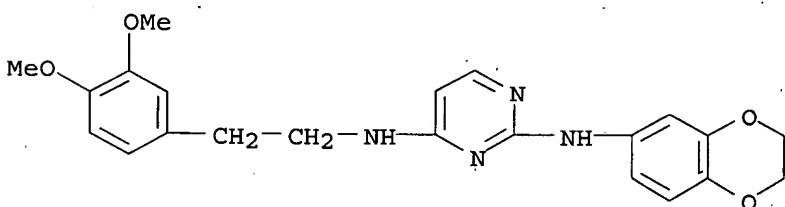
CRN 76-05-1
 CMF C2 H F3 O2



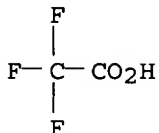
RN 691403-28-8 HCAPLUS
 CN 2,4-Pyrimidinediamine, N2-(2,3-dihydro-1,4-benzodioxin-6-yl)-N4-[2-(3,4-dimethoxyphenyl)ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691403-27-7
 CMF C22 H24 N4 O4

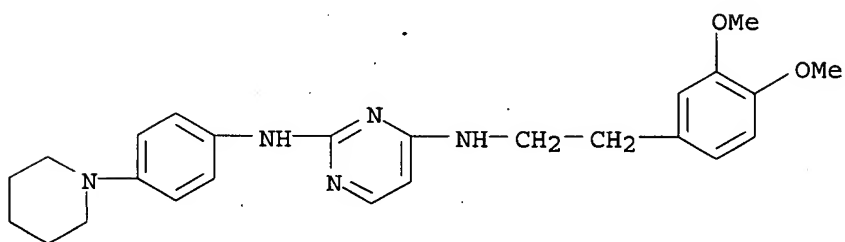


CM 2

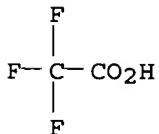
CRN 76-05-1
CMF C2 H F3 O2

RN 691403-30-2 HCAPLUS
 CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-[4-(1-piperidiny)phenyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691403-29-9
CMF C25 H31 N5 O2

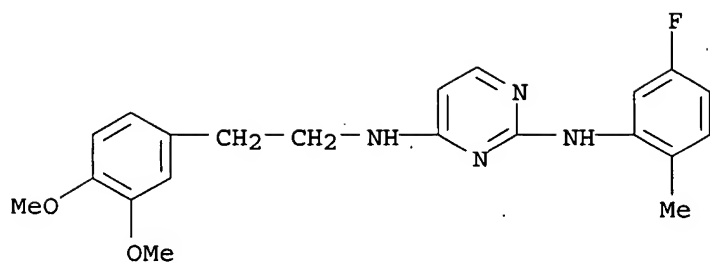
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 691403-32-4 HCAPLUS
 CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-(5-fluoro-2-methylphenyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

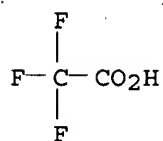
CRN 691403-31-3
CMF C21 H23 F N4 O2



CM 2

CRN 76-05-1

CMF C2 H F3 O2



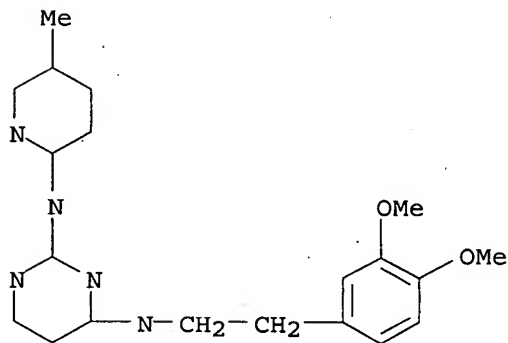
RN 691403-34-6 HCAPLUS

CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-(5-methyl-2-pyridinyl)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691403-33-5

CMF C20 H23 N5 O2

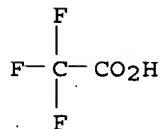


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1

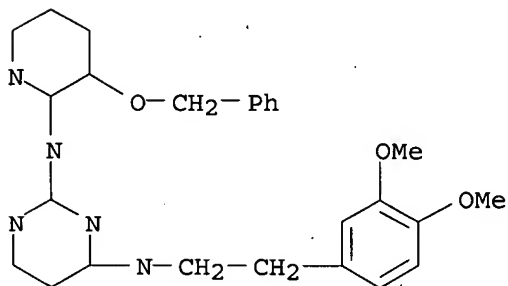
CMF C2 H F3 O2



RN 691403-36-8 HCAPLUS
 CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-[3-(phenylmethoxy)-2-pyridinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

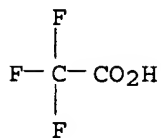
CRN 691403-35-7
 CMF C26 H27 N5 O3



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

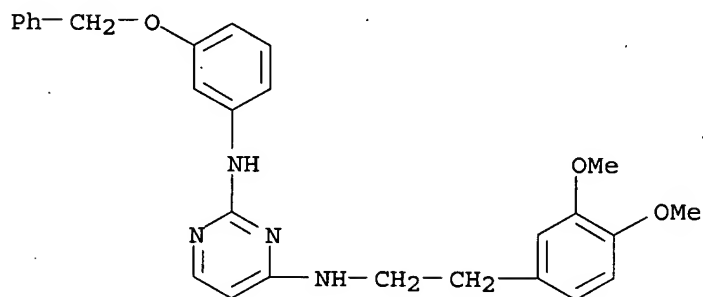
CRN 76-05-1
 CMF C2 H F3 O2



RN 691403-38-0 HCAPLUS
 CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-[3-(phenylmethoxy)phenyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

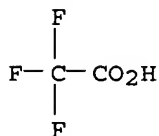
CM 1

CRN 691403-37-9
 CMF C27 H28 N4 O3



CM 2

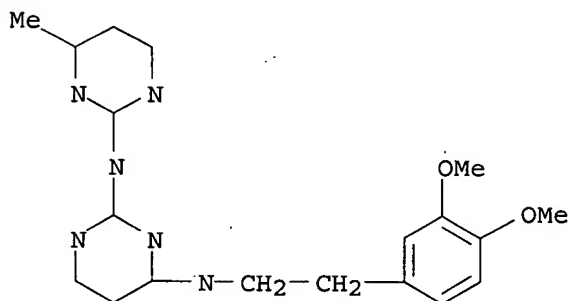
CRN 76-05-1
CMF C2 H F3 O2



RN 691403-41-5 HCAPLUS
CN 2,4-Pyrimidinediamine, N4-[2-(3,4-dimethoxyphenyl)ethyl]-N2-(4-methyl-2-pyrimidinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

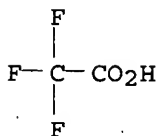
CRN 691403-40-4
CMF C19 H22 N6 O2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

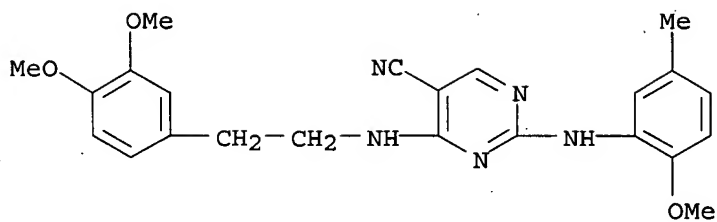
CRN 76-05-1
CMF C2 H F3 O2



RN 691405-34-2 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[(2-methoxy-5-methylphenyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

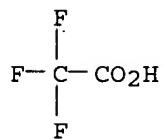
CRN 691405-33-1
CMF C23 H25 N5 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



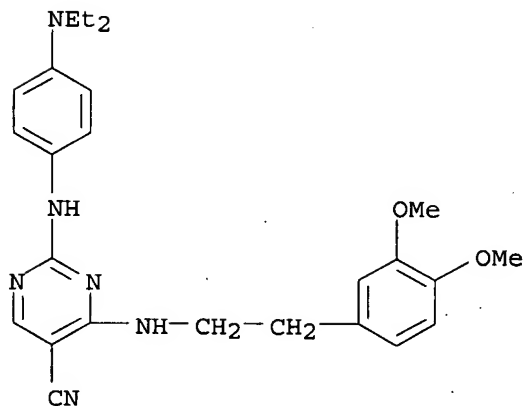
RN 691405-37-5 HCAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[[4-(diethylamino)phenyl]amino]-4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691405-36-4

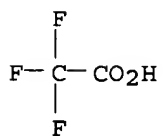
CMF C25 H30 N6 O2



CM 2

CRN 76-05-1

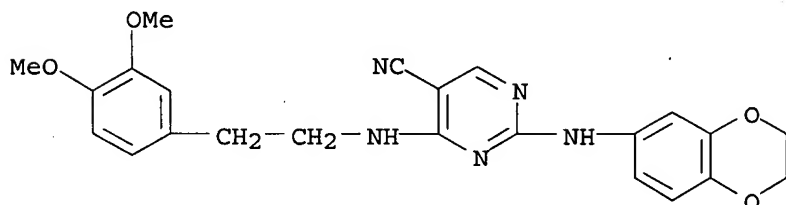
CMF C2 H F3 O2



RN 691405-39-7 HCAPLUS
 CN 5-Pyrimidinecarbonitrile, 2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

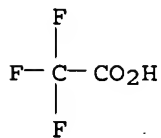
CM 1

CRN 691405-38-6
 CMF C23 H23 N5 O4



CM 2

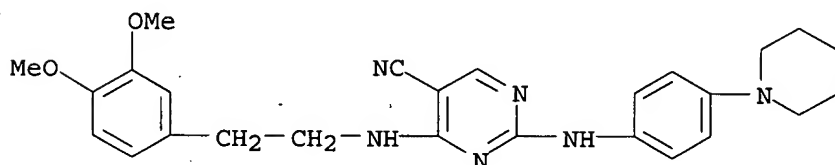
CRN 76-05-1
 CMF C2 H F3 O2



RN 691405-41-1 HCAPLUS
 CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[[4-(1-piperidiny)phenyl]amino]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

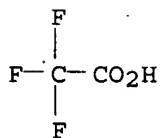
CM 1

CRN 691405-40-0
 CMF C26 H30 N6 O2



CM 2

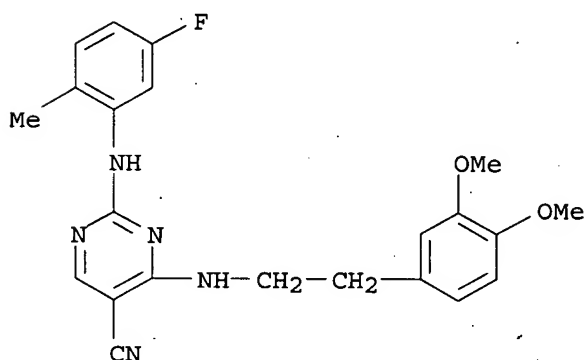
CRN 76-05-1
 CMF C2 H F3 O2



RN 691405-43-3 HCAPLUS
 CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[(5-fluoro-2-methylphenyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

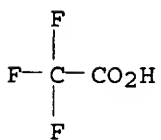
CM 1

CRN 691405-42-2
 CMF C22 H22 F N5 O2



CM 2

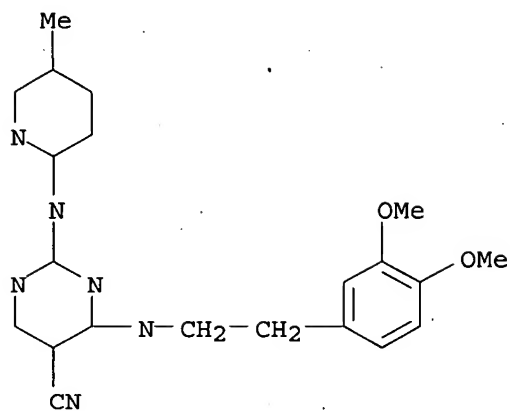
CRN 76-05-1
 CMF C2 H F3 O2



RN 691405-45-5 HCAPLUS
 CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[(5-methyl-2-pyridinyl)amino]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691405-44-4
 CMF C21 H22 N6 O2

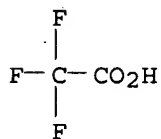


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1

CMF C2 H F3 O2



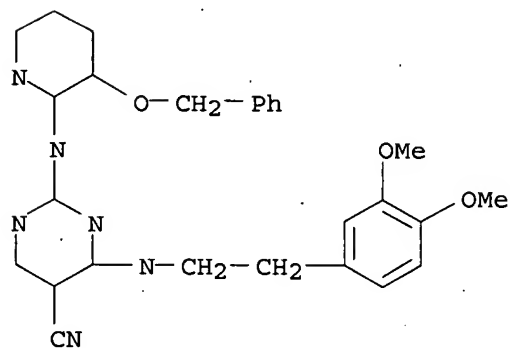
RN 691405-48-8 HCAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[[3-(phenylmethoxy)-2-pyridinyl]amino]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691405-47-7

CMF C27 H26 N6 O3

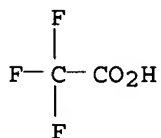


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 76-05-1

CMF C2 H F3 O2



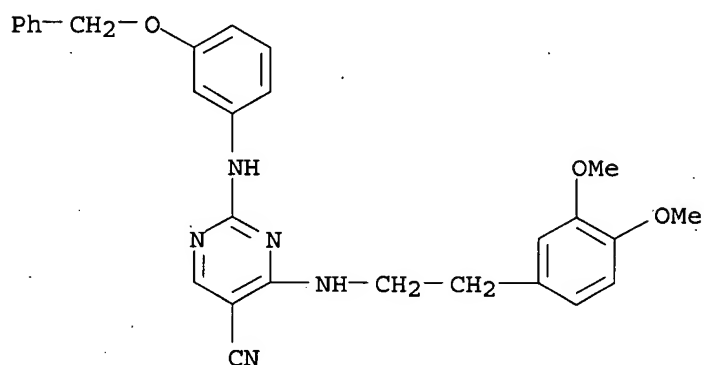
RN 691405-50-2 HCAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[[3-(phenylmethoxy)phenyl]amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691405-49-9

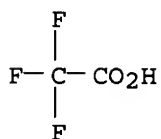
CMF C28 H27 N5 O3



CM 2

CRN 76-05-1

CMF C2 H F3 O2



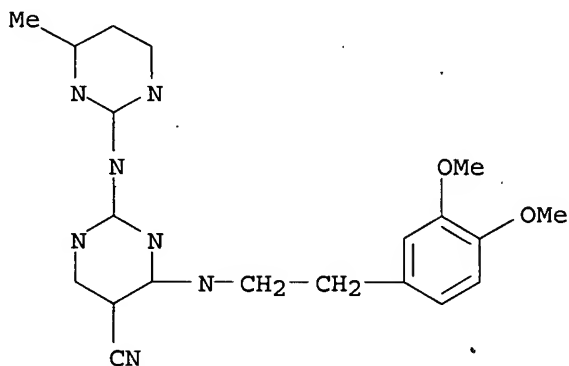
RN 691405-52-4 HCAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[(4-methyl-2-pyrimidinyl)amino]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 691405-51-3

CMF C20 H21 N7 O2

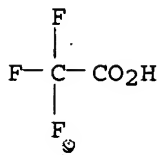


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

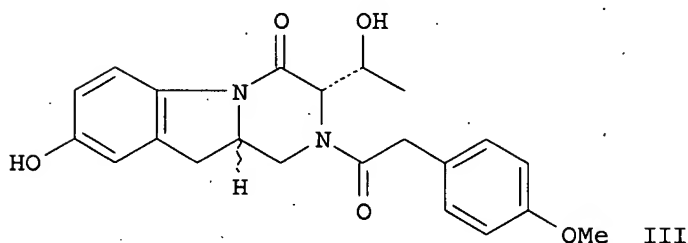
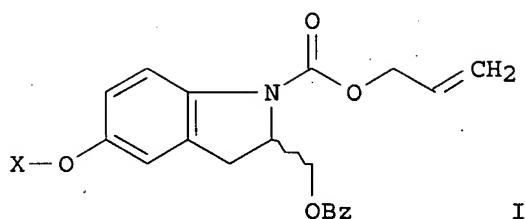
CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:986464 HCAPLUS
 DOCUMENT NUMBER: 140:163824
 TITLE: A Solid Phase Library Synthesis of Hydroxyindoline-Derived Tricyclic Derivatives by Mitsunobu Approach
 AUTHOR(S): Arya, Prabhat; Wei, Chang-Qing; Barnes, Michael L.; Daroszewska, Malgosia
 CORPORATE SOURCE: Steacie Institute for Molecular Sciences, Chemical Biology Program, National Research Council of Canada, Ottawa, ON, K1A 0R6, Can.
 SOURCE: Journal of Combinatorial Chemistry (2004), 6(1), 65-72
 CODEN: JCCHFF; ISSN: 1520-4766
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:163824
 GI



AB Hydroxyindoline-derived scaffold I [X = H, resin (II)] was synthesized with the goal of generating a library of indoline-based natural product-like tricyclic derivs. to be utilized as small-mol. chemical probes. The tricyclic ring was obtained by a Mitsunobu reaction of the N-nosyl amino acid conjugate with the primary hydroxyl group. The solid-phase synthesis was achieved by immobilizing I (X = H) onto the solid support giving II. II was then subjected to a series of reactions on solid phase, including the Mitsunobu reaction, leading to the desired indoline-derived tricyclic derivative, e.g., III. The final product has two diversity sites: (i) amino acid as the first diversity and (ii) amidation of the secondary amine for the second diversity. These two diversity sites were utilized in the library generation by IRORI split-and-mix approach.

IT 654060-03-4P

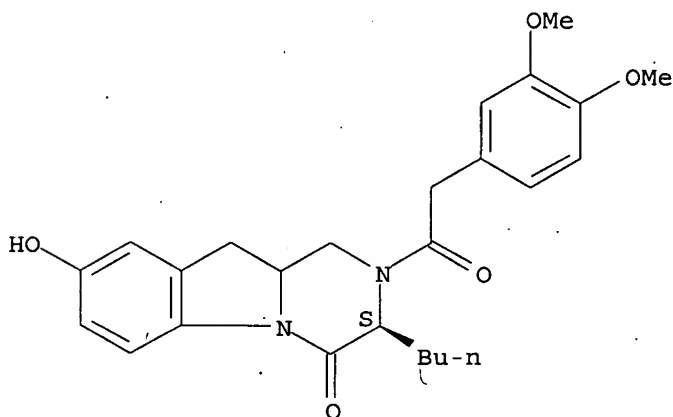
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(solid phase preparation of a library of indoline-derived tricyclic derivs. via coupling of amino acids to resin bound benzoyloxymethylindoline followed by intramol. Mitsunobu reaction and subsequent amidation with carboxylic acids)

RN 654060-03-4 HCAPLUS

CN Pyrazino[1,2-a]indol-4(1H)-one, 3-butyl-2-[(3,4-dimethoxyphenyl)acetyl]-2,3,10,10a-tetrahydro-8-hydroxy-, (3S)- (9CI) (CA INDEX NAME)

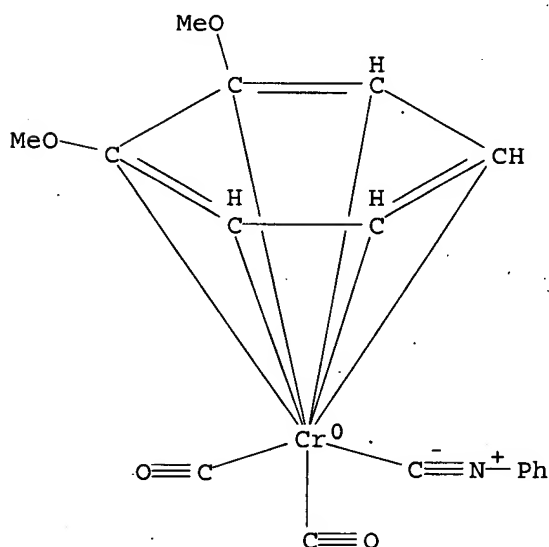
Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 12 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:772340 HCAPLUS
 DOCUMENT NUMBER: 139:396026
 TITLE: Polymer-Supported Haloarene Chromium Dicarbonyl Isonitrile Complexes: A Study of Their Synthesis and Reactivity
 AUTHOR(S): Baldoli, Clara; Maiorana, Stefano; Licandro, Emanuela; Casiraghi, Laura; Zinzalla, Giovanna; Seneci, Pierfausto; De Magistris, Elisabetta; Paio, Alfredo; Marchioro, Carla
 CORPORATE SOURCE: Dipartimento di Chimica Organica e Industriale, Istituto di Scienze e Tecnologie Molecolari, Centro di Eccellenza CISI, University of Milan and CNR, Milan, I-20133, Italy
 SOURCE: Journal of Combinatorial Chemistry (2003), 5(6), 809-813
 CODEN: JCCHFF; ISSN: 1520-4766
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:396026

AB Different arene $\text{Cr}(\text{CO})_3$ complexes were supported on a polystyrene isonitrile resin by photochem.-promoted replacement of a Cr carbonyl ligand by the NC group. The supported complexes proved to be stable and were successfully used for further transformations. In particular, the reactivity of dichlorobenzene complexes to different nucleophiles was studied and is comparable with that of the parent $\text{Cr}(\text{CO})_3$ complexes.
 IT 625851-72-1DP, hydroxymethylated polystyrene resin-supported
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and iodine-promoted oxidative cleavage reaction of polystyrene-supported haloarene-chromium complex)
 RN 625851-72-1 HCAPLUS
 CN Chromium, dicarbonyl[(1,2,3,4,5,6- η)-1,2-dimethoxybenzene] [(isocyano- κ C)benzene]- (9CI) (CA INDEX NAME).



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

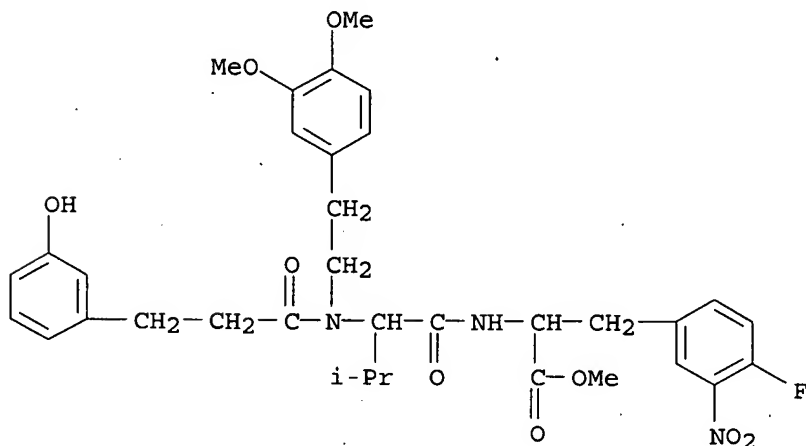
L17 ANSWER 13 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:746726 HCAPLUS
DOCUMENT NUMBER: 140:5292
TITLE: Rapid and diverse route to natural product-like biaryl
ether containing macrocycles
AUTHOR(S): Cristau, Pierre; Vors, Jean-Pierre; Zhu, Jieping
CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, CNRS,
Gif-sur-Yvette, 91198, Fr.
SOURCE: Tetrahedron (2003), 59(40), 7859-7870
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:5292
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

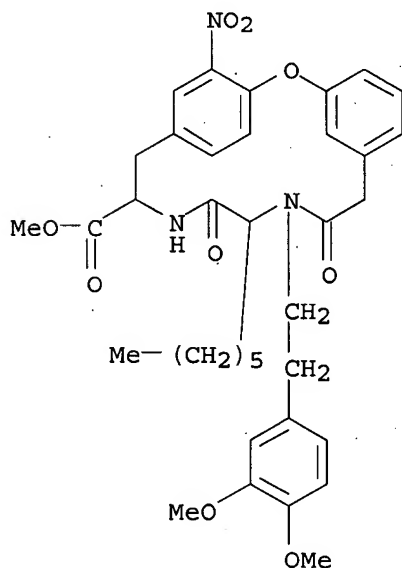
AB A two-step sequence involving an Ugi four-component reaction and an intramol. nucleophilic aromatic substitution (SNAr) has been developed for the rapid access to biaryl-ether containing macrocycles. For example, reacting heptanal with butylamine, (3-hydroxyphenyl)acetic acid, and isonitrile I in dry toluene in the presence of NH₄Cl gave dipeptide II. II was then cyclized using an intramol. SNAr sequence to give cyclic ether III as a mixture of 4 diastereomers. In the course of this study, we documented that ammonium chloride can promote the Ugi-4CR in non-polar aprotic solvent (toluene) without the interference of an alternative Passerini reaction. Solid phase synthesis of macrocycles by this two-step sequence was also developed using polymer (Wang resin) supported α -(4'-fluoro-3'-nitro)phenethyl isocyanoacetate as one of the inputs.

IT 389634-89-3P 604004-09-3P 627535-92-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of natural-product like biaryl ether macrocycles by solution and solid-phase Ugi reaction-intramol. nucleophilic aromatic substitution)

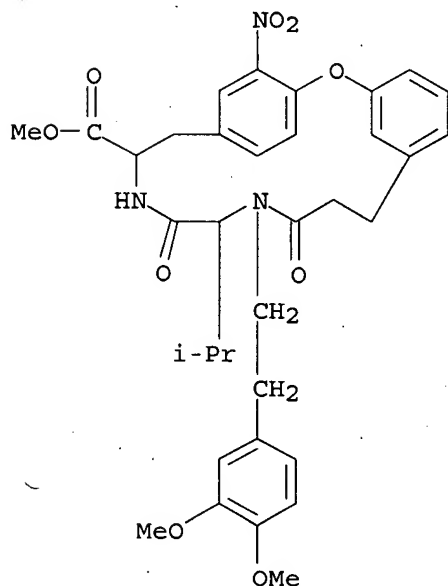
RN 389634-89-3 HCAPLUS
CN Phenylalanine, N-[2-(3,4-dimethoxyphenyl)ethyl]-N-[3-(3-hydroxyphenyl)-1-oxopropyl]valyl-4-fluoro-3-nitro-, methyl ester (9CI) (CA INDEX NAME)



RN 604004-09-3 HCAPLUS
 CN 2-Oxa-10,13-diazatricyclo[14.2.2.13,7]heneicosa-3,5,7(21),16,18,19-hexaene-14-carboxylic acid, 10-[2-(3,4-dimethoxyphenyl)ethyl]-11-hexyl-18-nitro-9,12-dioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 627535-92-6 HCAPLUS
 CN 2-Oxa-11,14-diazatricyclo[15.2.2.13,7]docosa-3,5,7(22),17,19,20-hexaene-15-carboxylic acid, 11-[2-(3,4-dimethoxyphenyl)ethyl]-12-(1-methylethyl)-19-nitro-10,13-dioxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 14 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:714485 HCAPLUS

DOCUMENT NUMBER: 140:271138
 TITLE: Diastereomeric Process Control in the Synthesis of
 2'-O-(2-Methoxyethyl) Oligoribonucleotide
 Phosphorothioates as Antisense Drugs
 AUTHOR(S): Ravikumar, Vasulinga T.; Cole, Douglas L.
 CORPORATE SOURCE: Isis Pharmaceuticals, Carlsbad, CA, 92008, USA
 SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2003
), 22(5-8), 1639-1645
 CODEN: NNNAFY; ISSN: 1525-7770
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Coupling of 2'-O-methoxyethyl-substituted nucleoside
 phosphoramidites to 5'-hydroxyl group of a nucleoside or
 nucleotide on solid support is under stereochem. process control
 and is independent of scale, concentration, synthesizer, ratio of amidite
 diastereomers, solid support etc. However, activators and phosphate
 protecting groups do play a role in influencing the ratio of
 phosphorothioate diesters obtained by sulfurization of phosphite
 triesters.

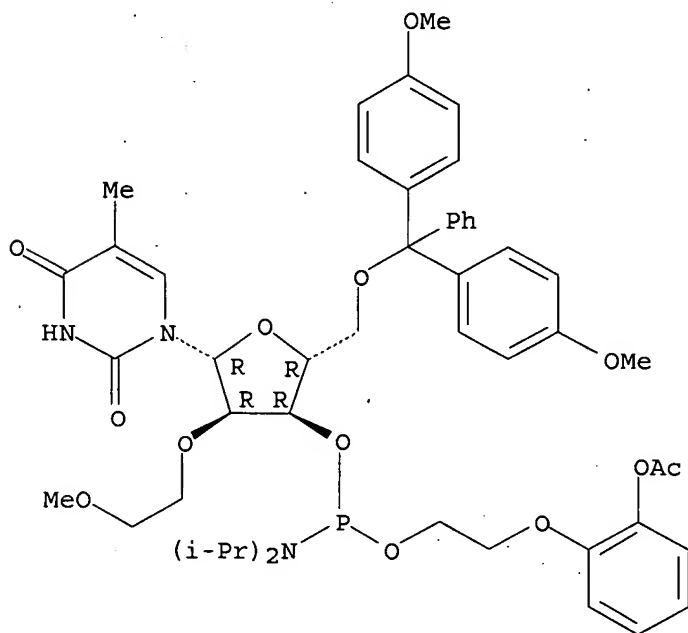
IT 674798-38-0P 674798-40-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (diastereomeric process control in synthesis of methoxyethyl
 oligoribonucleotide phosphorothioates as antisense drugs)

RN 674798-38-0 HCAPLUS

CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(2-methoxyethyl)-5-
 methyl-, 3'-[2-[2-(acetyloxy)phenoxy]ethyl bis(1-
 methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

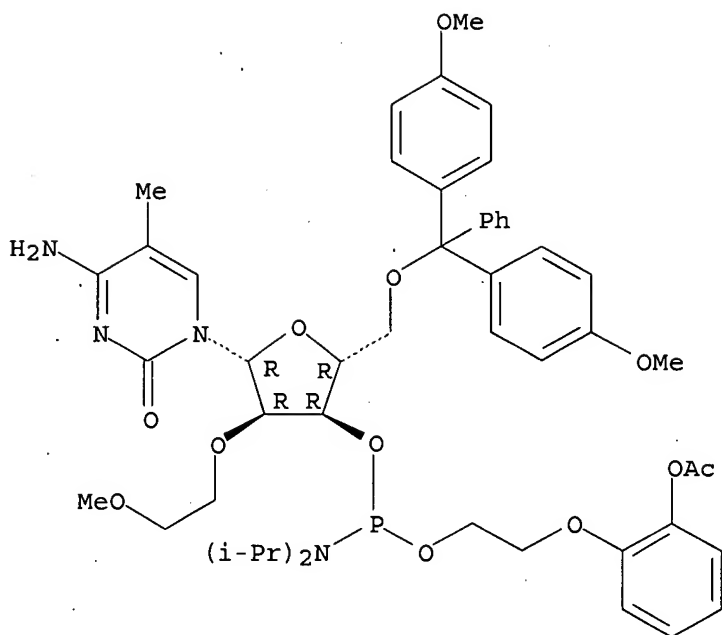
Absolute stereochemistry.



RN 674798-40-4 HCAPLUS

CN Cytidine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(2-methoxyethyl)-5-
 methyl-, 3'-[2-[2-(acetyloxy)phenoxy]ethyl bis(1-
 methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d 117 ibib abs hitstr 15-28

L17 ANSWER 15 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:714432 HCAPLUS

DOCUMENT NUMBER: 140:287649

TITLE: Understanding High Diastereomeric Discrimination in Formation of Oligoribonucleotide Phosphorothioate Linkages: The First Study of pKa-Dependent Activation in Solid-Supported Coupling of 2'-O-Substituted Ribonucleoside Phosphoramidites

AUTHOR(S): Ravikumar, Vasulinga T.; Cole, Douglas L.
CORPORATE SOURCE: Isis Pharmaceuticals, Carlsbad, CA, 92009, USA
SOURCE: Nucleosides, Nucleotides & Nucleic Acids (2003), 22(5-8), 1415-1419

CODEN: NNNAFY; ISSN: 1525-7770

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:287649

AB Activation of 2'-O-substituted ribonucleoside phosphoramidites with various activators during solid-supported synthesis of phosphorothioate oligonucleotides was studied. The Rp:Sp diastereomeric composition of resulting phosphorothioate linkage dependent on pKa of activator utilized for coupling.

IT 674798-38-0

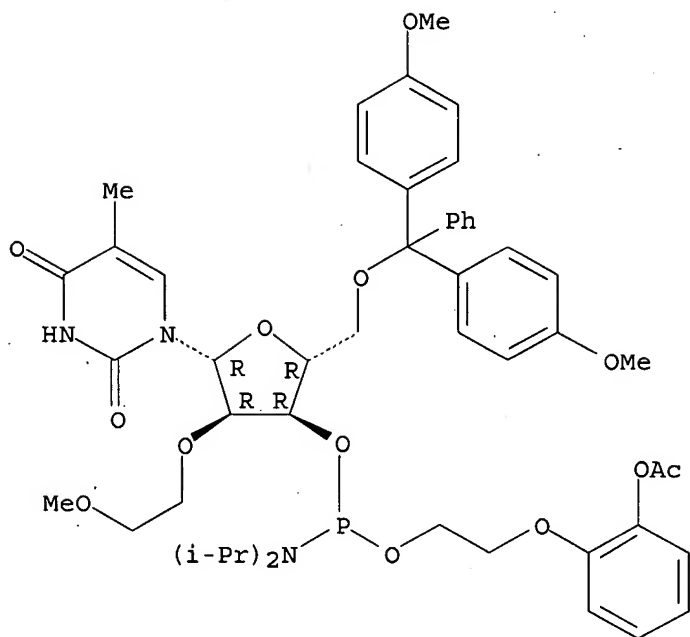
RL: RCT (Reactant); RACT (Reactant or reagent)

(understanding high diastereomeric discrimination in formation of oligoribonucleotide phosphorothioate linkages and study of pKa-dependent activation in solid-supported coupling of substituted ribonucleoside phosphoramidites)

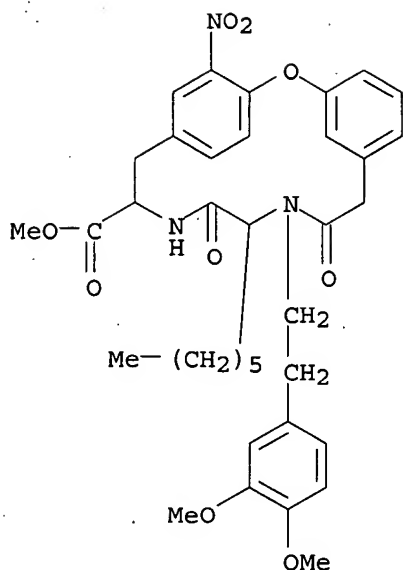
RN 674798-38-0 HCAPLUS

CN Uridine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-2'-O-(2-methoxyethyl)-5-methyl-, 3'-[2-[2-(acetyloxy)phenoxy]ethyl bis(1-methylethyl)phosphoramidite] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 16 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2003:495132 HCAPLUS
 DOCUMENT NUMBER: 139:277143
 TITLE: Solid-phase synthesis of natural product-like macrocycles by a sequence of Ugi-4CR and SNAr-based cycloetherification
 AUTHOR(S): Cristau, Pierre; Vors, Jean-Pierre; Zhu, Jieping
 CORPORATE SOURCE: CNRS, Institut de Chimie des Substances Naturelles, Gif-sur-Yvette, 91198, Fr.
 SOURCE: Tetrahedron Letters (2003), 44(30), 5575-5578
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:277143
 AB An on-resin Ugi four-component reaction followed by an intramol. nucleophilic aromatic substitution (SNAr) has been developed for the rapid access to biaryl-ether containing macrocycles. Supported isocyanide was prepared and used together with heptanal, butylamine, and 3-hydroxyphenylacetic acid for on-resin Ugi four-component reaction.
 IT 604004-09-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (solid-phase peptide synthesis of macrocycles from prepared supported isocyanide by Ugi four-component reaction followed by nucleophilic aromatic substitution-based cycloetherification)
 RN 604004-09-3 HCAPLUS
 CN 2-Oxa-10,13-diazatricyclo[14.2.2.13,7]heneicosa-3,5,7(21),16,18,19-hexaene-14-carboxylic acid, 10-[2-(3,4-dimethoxyphenyl)ethyl]-11-hexyl-18-nitro-9,12-dioxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 17 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:178448 HCAPLUS

DOCUMENT NUMBER: 138:354164

TITLE: Solid-Phase Synthesis of Nucleoside Analogs

AUTHOR(S): Epple, Robert; Kudirka, Romas; Greenberg, William A.

CORPORATE SOURCE: Genomics Institute of the Novartis Research Foundation, San Diego, CA, 92121, USA

SOURCE: Journal of Combinatorial Chemistry (2003), 5(3), 292-310

CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:354164

AB The synthesis of a 25 000 member library of nucleoside analogs as discrete compds. in milligram quantities is described. The use of the Nanokan technol. developed by IRORI (Discovery Partners International) together with macroporous solid support allowed us to develop a highly reliable and practical synthetic route for the high-throughput derivatization of both the pyrimidine and purine nucleoside scaffold. A 2',3'-acetal linkage of the scaffolds to the solid support proved to be stable enough for the chemical transformations employed, yet labile enough for mild cleavage conditions to yield final products in high purity. The publication represents an example for combining synthetic organic chemical on advanced scaffolds with the latest technologies of combinatorial chemical in order to provide both industrial and academic institutions with compds. in high number and quality, thereby accelerating the search for novel biol. targets and drug development.

IT 518316-16-0P

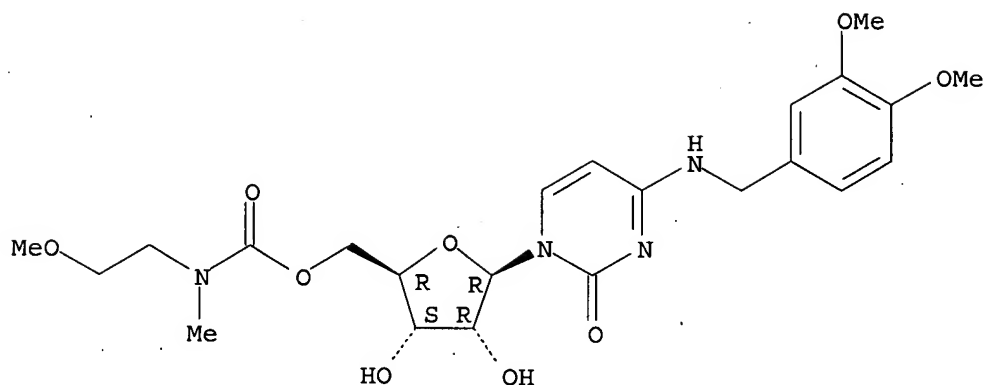
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(solid phase and combinatorial library synthesis of nucleoside analogs)

RN 518316-16-0 HCAPLUS

CN Cytidine, N-[(3,4-dimethoxyphenyl)methyl]-, 5'-[(2-methoxyethyl)methylcarbamate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 83 THERE ARE 83 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 18 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:114257 HCAPLUS

DOCUMENT NUMBER: 138:287628

TITLE: Solution- and Solid-Phase Parallel Synthesis of 4-Alkoxy-Substituted Pyrimidines with High Molecular Diversity

AUTHOR(S): Font, David; Heras, Montserrat; Villalgordo, Jose M.

CORPORATE SOURCE: Departament de Química, Facultat de Ciències, Universitat de Girona, Girona, E-17071, Spain

SOURCE: Journal of Combinatorial Chemistry (2003), 5(3), 311-321

CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:287628

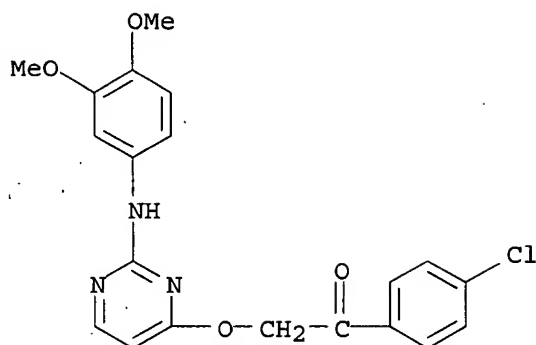
AB A simple and straightforward methodol. toward the synthesis of novel 2,6-disubstituted-4-alkoxypyrimidine derivs. has been developed. This methodol., initially developed in solution, can be perfectly adapted to the solid support under analogous conditions, taking full advantage of automated parallel synthesis systems. This successful methodol. benefits from the key role played by the thioether linkage placed at the 2-position in a double manner: on one side, the steric effect exerted by the thioether linkage is likely to be responsible for the very high observed selectivity toward the formation of the O-alkylation products. On the other side, this sulfur linkage can serve not only as a robust point of attachment for the heterocycle, stable to a number of reaction conditions, but also as a means of introducing a new element of diversity through ipso-substitution reaction with a variety of different N-nucleophiles.

IT 503855-91-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (solution- and solid-phase parallel synthesis of 4-alkoxypyrimidines with high mol. diversity)

RN 503855-91-2 HCAPLUS

CN Ethanone, 1-(4-chlorophenyl)-2-[[2-[(3,4-dimethoxyphenyl)amino]-4-pyrimidinyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 19 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:5916 HCAPLUS

DOCUMENT NUMBER: 138:73466

TITLE: Preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of nucleic acids

INVENTOR(S): Serafinowski, Pawel Jerzy; Garland, Peter Bryan

PATENT ASSIGNEE(S): The Institute of Cancer Research, UK

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

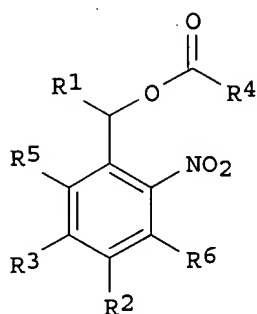
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003000644	A1	20030103	WO 2002-GB2896	20020621 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002314335	A1	20030108	AU 2002-314335	20020621 <--
EP 1399412	A1	20040324	EP 2002-740905	20020621 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004242653	A1	20041202	US 2004-481707	20040716 <--
PRIORITY APPLN. INFO.:				
			GB 2001-15231	A 20010621
			GB 2001-22760	A 20010921
			WO 2002-GB2896	W 20020621

OTHER SOURCE(S): MARPAT 138:73466

GI



I

AB Nucleotides I wherein: R1 is selected from hydrogen, aryl or substituted aryl, aryloxy or substituted aryloxy, or an unsubstituted or substituted heterocyclic group; R2 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or a nitro group; R3 is selected from hydrogen, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, or an unsubstituted or substituted heterocyclic group; R4 is an alkyl group substituted with one or more halogen substituents; R5 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, amino or substituted amino, a nitro group or an unsubstituted or substituted heterocyclic group; and, R6 is selected from hydrogen, halogen, alkyl or substituted alkyl, alkoxy or substituted alkoxy, aryl or substituted aryl, aryloxy or substituted aryloxy, or amino or substituted amino, or an unsubstituted or substituted heterocyclic group, which are capable of generating acid on photolysis are disclosed, and the uses of these compds., especially for deprotecting the termini of nucleic acid mols. or peptides during synthesis of arrays. The compds. described herein may be employed in the detritylation of 5'-O-dimethoxytrityl (DMT) protected nucleotides by photolyzing the compds. to generate an acid capable of removing the DMT group allowing oligonucleotide arrays to be synthesized using readily available 5'-O-DMT-nucleoside-3'-O-phosphoramidite monomers conventionally used in solid phase nucleic acid synthesis. A method of avoiding the effects of stray light in projection lithog. techniques is also disclosed. Thus, α -phenyl-4,5-dimethoxy-2,6-dinitrobenzyltrichloroacetate was prepared and used in DNA synthesis.

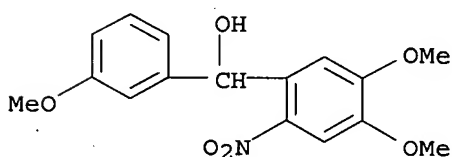
IT 479637-48-4P 479637-49-5P 479637-66-6P
479637-67-7P 479637-68-8P 479637-75-7P
479637-76-8P 479637-77-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

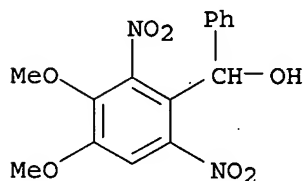
(preparation of nucleotide photolabile esters capable of generating acid on photolysis in solid phase synthesis of DNA)

RN 479637-48-4 HCAPLUS

CN Benzenemethanol, 4,5-dimethoxy- α -(3-methoxyphenyl)-2-nitro- (9CI)
(CA INDEX NAME)

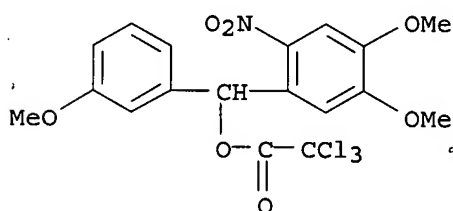


RN 479637-49-5 HCAPLUS

CN Benzenemethanol, 3,4-dimethoxy-2,6-dinitro- α -phenyl- (9CI) (CA INDEX NAME)

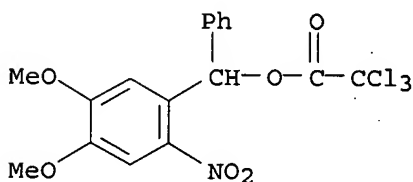
RN 479637-66-6 HCAPLUS

CN Acetic acid, trichloro-, (4,5-dimethoxy-2-nitrophenyl) (3-methoxyphenyl)methyl ester (9CI) (CA INDEX NAME)



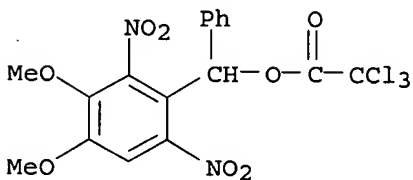
RN 479637-67-7 HCAPLUS

CN Acetic acid, trichloro-, (4,5-dimethoxy-2-nitrophenyl)phenylmethyl ester (9CI) (CA INDEX NAME)



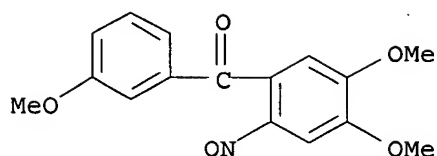
RN 479637-68-8 HCAPLUS

CN Acetic acid, trichloro-, (3,4-dimethoxy-2,6-dinitrophenyl)phenylmethyl ester (9CI) (CA INDEX NAME)



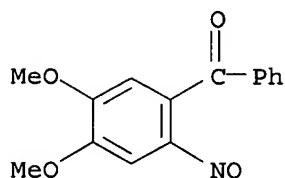
RN 479637-75-7 HCAPLUS

CN Methanone, (4,5-dimethoxy-2-nitrosophenyl) (3-methoxyphenyl)- (9CI) (CA INDEX NAME)



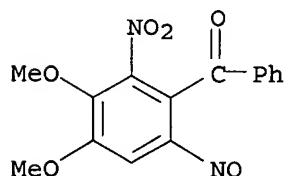
RN 479637-76-8 HCAPLUS

CN Methanone, (4,5-dimethoxy-2-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



RN 479637-77-9 HCAPLUS

CN Methanone, (3,4-dimethoxy-2-nitro-6-nitrosophenyl)phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 20 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:148 HCAPLUS

DOCUMENT NUMBER: 138:205020

TITLE: Novel Orthogonal Strategy toward Solid-Phase Synthesis of 1,3,5-Substituted Triazines

AUTHOR(S): Bork, Jacqueline T.; Lee, Jae Wook; Khersonsky, Sonya M.; Moon, Ho-Sang; Chang, Young-Tae

CORPORATE SOURCE: Department of Chemistry, New York University, New York, NY, 10003, USA

SOURCE: Organic Letters (2003), 5(2), 117-120

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205020

AB A library of triamino-1,3,5-triazines are prepared on solid-phase using the oxidation of benzylthiotriazines to benzylsulfonyltriazines followed by nucleophilic substitution of the benzylsulfonyltriazines with amines as the key steps. Attachment of a primary amine to a formyl-substituted polystyrene (PAL) resin, addition of a dichloro(benzylthio)-1,3,5-triazine to the resin-bound primary amine, substitution of the chlorine atom with an amine, oxidation of the benzylthio moiety, substitution of the newly generated benzylsulfonyl moiety with a second amine, and resin cleavage with trifluoroacetic acid in methylene chloride provides a 96-member triamino-1,3,5-triazine library in 71-99% purities. A set of resin-bound triazines with chloro and benzylsulfonyl moieties are reacted with a set of 30 amines to compare the use of

amino-substituted chlorotriazines, benzylthio-substituted chlorotriazines, and amino-substituted benzylsulfonyltriazines in substitution reactions with amines; substitution reactions of either amino-substituted sulfonyltriazines or benzylthio-substituted chlorotriazines gave the aminotriazine products in higher purities than reactions of amines with amino-substituted chlorotriazines.

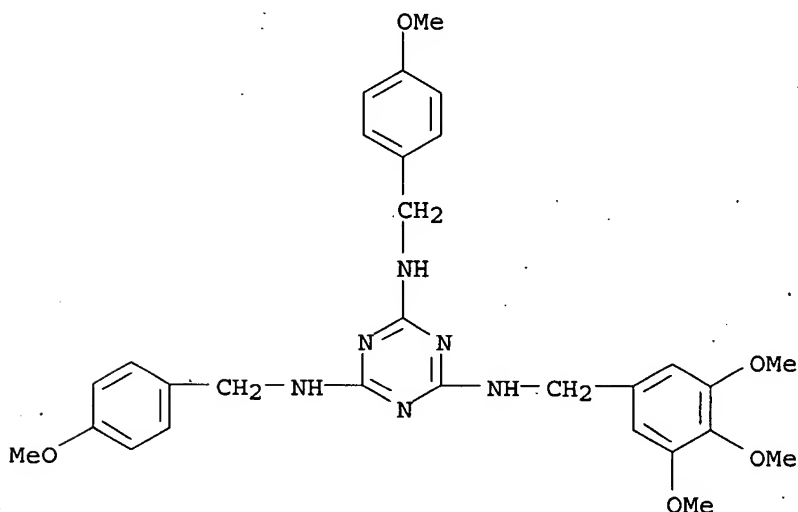
IT 500222-88-8P 500223-07-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(comparison of the purities of aminotriazines derived from substitution reactions of chlorotriazines and sulfonyltriazines on solid phase)

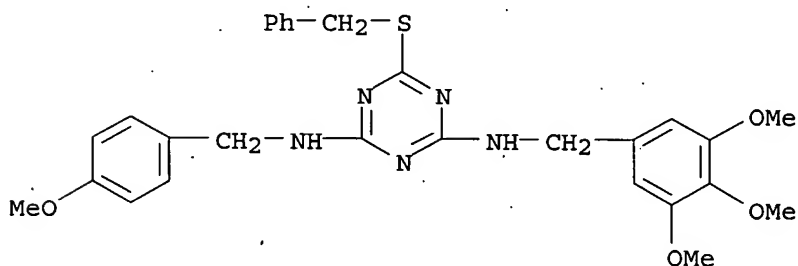
RN 500222-88-8 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N,N'-bis[(4-methoxyphenyl)methyl]-N''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 500223-07-4 HCAPLUS

CN 1,3,5-Triazine-2,4-diamine, N-[(4-methoxyphenyl)methyl]-6-[(phenylmethyl)thio]-N'-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



IT 500223-38-1P 500223-50-7P 500223-62-1P

500223-74-5P 500223-86-9P 500223-98-3P

500224-11-3P 500224-23-7P

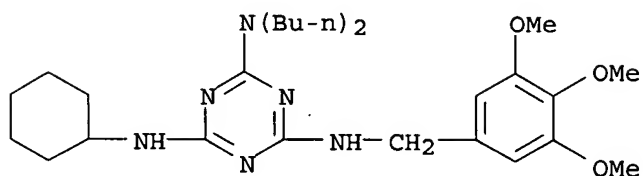
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(preparation of a library of triamino-1,3,5-triazines on solid phase using the oxidation and substitution reactions of benzylthio-1,3,5-triazines as key steps)

RN 500223-38-1 HCAPLUS

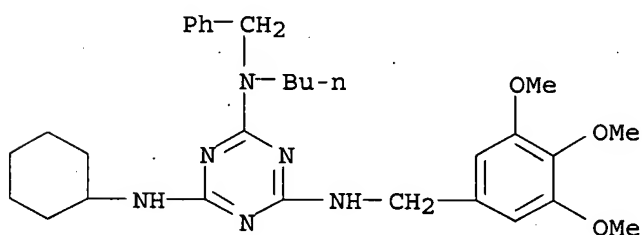
CN 1,3,5-Triazine-2,4,6-triamine, N,N-dibutyl-N'-cyclohexyl-N''-[(3,4,5-

trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



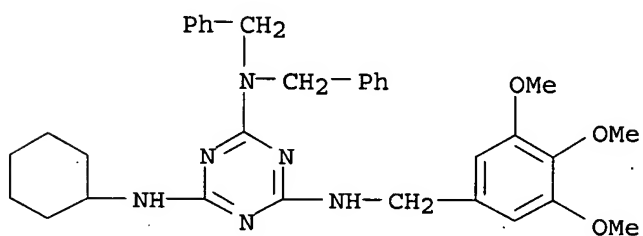
RN 500223-50-7 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-butyl-N'-cyclohexyl-N-(phenylmethyl)-N'''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



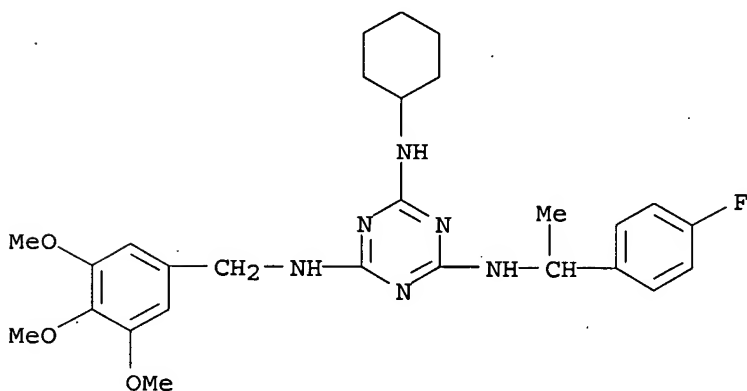
RN 500223-62-1 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N'-cyclohexyl-N,N-bis(phenylmethyl)-N'''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



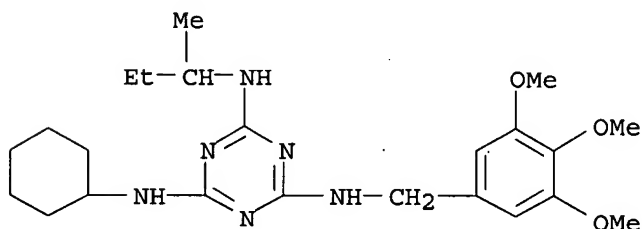
RN 500223-74-5 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-cyclohexyl-N'-[1-(4-fluorophenyl)ethyl]-N'''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



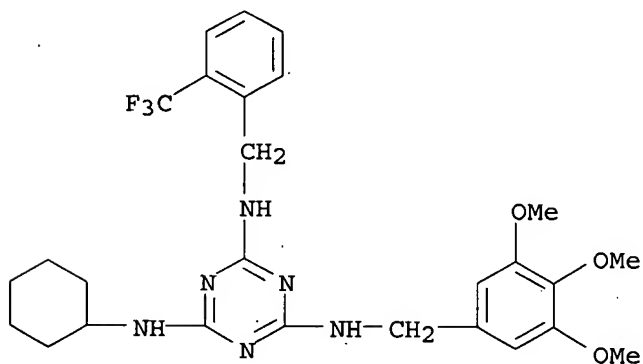
RN 500223-86-9 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-cyclohexyl-N'-(1-methylpropyl)-N''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



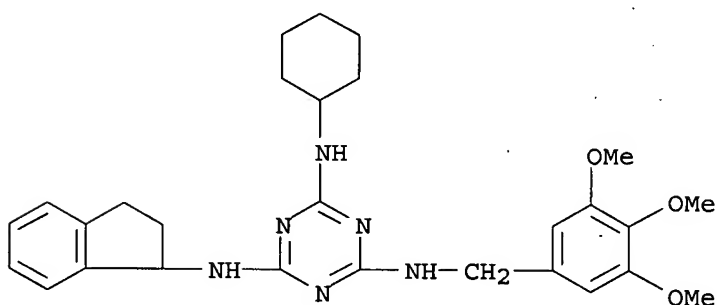
RN 500223-98-3 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-cyclohexyl-N'-[[2-(trifluoromethyl)phenyl]methyl]-N''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



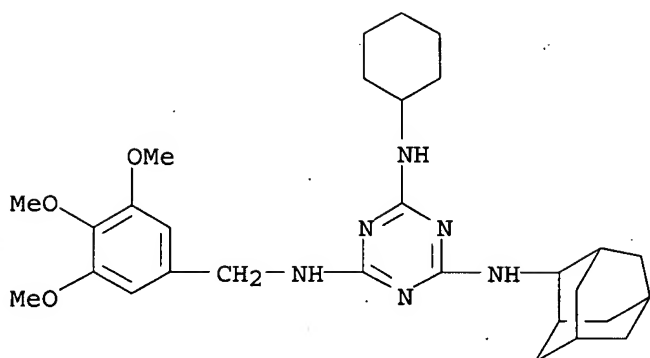
RN 500224-11-3 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-cyclohexyl-N'-(2,3-dihydro-1H-inden-1-yl)-N''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 500224-23-7 HCAPLUS

CN 1,3,5-Triazine-2,4,6-triamine, N-cyclohexyl-N'-tricyclo[3.3.1.1^{3,7}]dec-2-yl-N''-[(3,4,5-trimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 21 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:608591 HCAPLUS

DOCUMENT NUMBER: 137:294854

TITLE: Combinatorial Synthetic Design. Solution and Polymer-Supported Synthesis of Heterocycles via Intramolecular Aza Diels-Alder and Imino Alcohol Cyclizations

AUTHOR(S): Spaller, Mark R.; Thielemann, Wolfgang T.; Brennan, Paul E.; Bartlett, Paul A.

CORPORATE SOURCE: Center for New Directions in Organic Synthesis, University of California, Berkeley, CA, 94720-1460, USA

SOURCE: Journal of Combinatorial Chemistry (2002), 4(5), 516-522
CODEN: JCCHFF; ISSN: 1520-4766

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:294854

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Solution-phase and polymer-bound cyclization reactions are presented as a method for the stereoselective preparation of tetrahydroquinolines and tetrahydrobenzoxazepines with multiple points of variation as a potential method for combinatorial synthesis. Aldehydes connected to pendant alkenes undergo condensation with aromatic amines to give iminium ions which can either react intramol. by aza-Diels-Alder cycloaddn. reactions with pendant alkenes to give fused tetrahydroquinolines such as pyrroloquinoline I or intermolecularly with amino alcs. to give fused pyrrolidinones such as II. The stepwise nature of the cyclizations allows the reactivity to be varied through the presence or absence of external nucleophiles. Salicylaldehyde-derived aldehydes, amides and esters of glyoxalic acid, and aldehydes derived from L-amino acids are used as the aldehyde components; this allows potential variability at the aldehyde, linker, and alkene moieties. Aza-Diels-Alder cycloaddn. reactions give products with up to four stereocenters; the products of cycloaddn. are racemic, even when aldehydes derived from L-amino acids are used as aldehyde substrates. Addition of amino alcs. also gives racemic product except when D- or L-alaninol is used as the amino alc. component. The aza-Diels-Alder cycloaddn. of the aminoaldehydes is adapted and

optimized for solid phase synthesis.

IT 468762-30-3

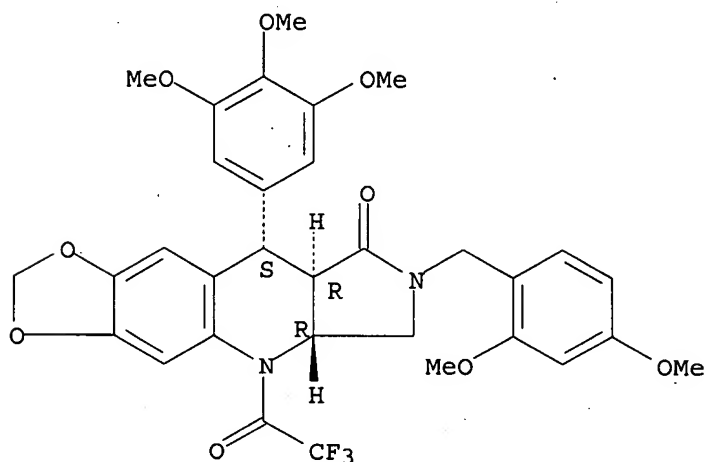
RL: PRP (Properties)

(crystal structures of compds. related to the stereoselective preparation of fused tetrahydroquinolines by condensation of aromatic amines with alkene-containing aldehydes followed by formal aza-Diels-Alder cycloaddn.)

RN 468762-30-3 HCAPLUS

CN 8H-1,3-Dioxolo[4,5-g]pyrrolo[3,4-b]quinolin-8-one, 7-[(2,4-dimethoxyphenyl)methyl]-5,5a,6,7,8a,9-hexahydro-5-(trifluoroacetyl)-9-(3,4,5-trimethoxyphenyl)-, (5aR,8aR,9S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 468762-18-7P

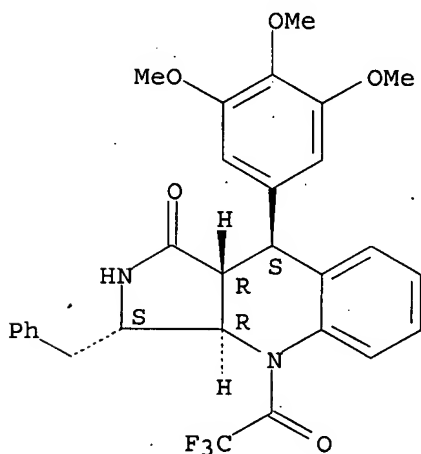
RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective solid-phase preparation of fused tetrahydroquinolines by condensation of aromatic amines with alkene-containing aldehydes followed by formal aza-Diels-Alder cycloaddn. and its use in combinatorial synthesis)

RN 468762-18-7 HCAPLUS

CN 1H-Pyrrolo[3,4-b]quinolin-1-one, 2,3,3a,4,9,9a-hexahydro-3-(phenylmethyl)-4-(trifluoroacetyl)-9-(3,4,5-trimethoxyphenyl)-, (3R,3aS,9R,9aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

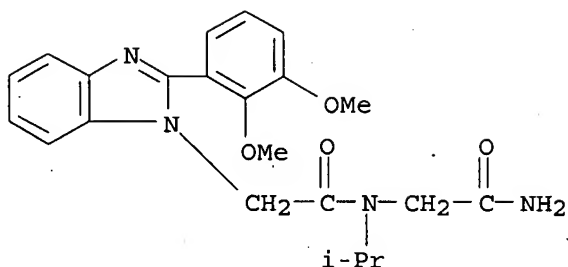
L17 ANSWER 22 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:536587 HCAPLUS
DOCUMENT NUMBER: 137:232595
TITLE: New Efficient Route for Solid-Phase
Synthesis of Benzimidazole Derivatives
AUTHOR(S): Akamatsu, Hisashi; Fukase, Koichi; Kusumoto, Shoichi
CORPORATE SOURCE: Department of Chemistry Graduate School of Science,
Osaka University, Osaka, 560-0043, Japan
SOURCE: Journal of Combinatorial Chemistry (2002),
4(5), 475-483
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232595
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Benzimidazoleacetamides such as I [R = H, Me, Cl, O₂N, CO₂H; R₁ = H, Me, Cl; R₂ = H, Me; R₃ = EtCH₂, Me₂CH, PhCH₂; R₃ = 2-MeC₆H₄, 3-MeC₆H₄, 4-MeC₆H₄, 2,4-Me₂C₆H₃, 4-Me₂CHCH₂C₆H₄, 4-Me₃CC₆H₄, 3-F₃CC₆H₄, 4-PhC₆H₄, 4-(2-pyridyl)C₆H₄, 3-ClC₆H₄, 2-Cl-6-FC₆H₃, 2-O₂N-5-ClC₆H₃, 4-(AcNH)C₆H₄, 4-Me₂NC₆H₄, 4-FC₆H₄, 3-O₂NC₆H₄, 4-F₃CC₆H₄, 2-ClC₆H₄, 2,3-Cl₂C₆H₃, Ph, 4-MeOC₆H₄, 2,3-(MeO)₂C₆H₃, 2-pyridyl, 3-pyridyl, 2-furyl, 2-pyrrolyl, 2-thienyl, 3-thienyl], imidazopyridineacetamides such as II and III (R₄ = 3-O₂NC₆H₄, Ph, 4-MeOC₆H₄) (4-aza and 5-azabenzimidazoles), and purineacetamides IV (R₅ = 3-O₂NC₆H₄, Ph, 4-MeOC₆H₄) containing peptoid linkers were prepared by a solid-phase synthesis from bromoacetic acid, primary amines, 1,2-benzenediamines, and aryl aldehydes. Deprotection of an Fmoc-amino resin with piperidine followed by acylation with bromoacetic acid and diisopropyl carbodiimide, nucleophilic substitution of the bromine with propylamine, isopropylamine, and benzylamine, and acylation of the secondary amine with bromoacetic acid and diisopropyl carbodiimide gives a resin-bound α -bromoamide PNHCOCH₂NRCOCH₂Br (P = polymer support; R = EtCH₂, Me₂CH, PhCH₂). Addition of 1,2-benzenediamines to the resin-bound α -bromoamide followed by addition of aryl aldehydes and heating in toluene at 50° and cleavage from the resin with trifluoroacetic acid give I. If 2,3-pyridinediamine, 3,4-pyridinediamine, or 4,5-pyrimidinediamine are used instead of 1,2-benzenediamines, fused azabenzimidazoles II and III, and purineacetamides IV are obtained. 4-Nitro-1,2-benzenediamine and 3,4-diaminobenzoic acid undergo regioselective cyclocondensations on solid-phase to give 6-substituted benzimidazoleacetamides while 4-chloro-1,2-benzenediamine and 4-methyl-1,2-benzenediamines both give mixts. of regioisomers.

IT 459439-28-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of substituted benzimidazoles on solid phase
by the condensation of aryl diamines with resin-bound
 α -bromoamides followed by cyclocondensation with aryl aldehydes
and resin cleavage)

RN 459439-28-2 HCAPLUS
CN 1H-Benzimidazole-1-acetamide, N-(2-amino-2-oxoethyl)-2-(2,3-dimethoxyphenyl)-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17. ANSWER 23 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:481310 HCAPLUS

DOCUMENT NUMBER: 137:216923

TITLE: Iron-Assisted Nucleophilic Aromatic Substitution on Solid Phase

AUTHOR(S): Ruhland, Thomas; Bang, Kia S.; Andersen, Kim

CORPORATE SOURCE: Department of Combinatorial Chemistry, Medicinal Chemistry Research, H. Lundbeck A/S, Valby, DK-2500, Den.

SOURCE: Journal of Organic Chemistry (2002), 67(15), 5257-5268

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:216923

AB Iron-assisted SNAr reactions are performed for the first time on solid phase and used in the preparation of a library of 36 unsym. substituted phenylpiperazines and phenyl-1,4-diazepanes. Piperazine and 1,4-diazepane are attached to Merrifield resin; addition of (chlorophenyl)(cyclopentadienyl)iron hexafluorophosphates yields resin-bound iron arene complexes. In the key step, the resin-bound iron arene complexes undergo SNAr reactions with salts of nucleophiles such as 3-methoxybenzyl alc., 2-methoxybenzyl alc., cyclohexanethiol, 1-adamantanethiol, 3-methoxybenzenethiol, 4-(tert-butyl)phenylselenol, diphenylphosphine, diphenylphosphinylselenol, and a dimethyldihydroanthracenylpiperidine to give a variety of products. Treatment of the resin-bound substituted arylpiperidine iron arene complexes with 1,10-phenanthroline and irradiation yields the resin-bound products and soluble phenanthroline iron complexes which can be easily removed; the reaction progress is easily monitored by the appearance of a red color in the reaction (the soluble iron phenanthroline complex). Resin cleavage with Me chloroformate yields 4-(methoxycarbonyl)-1-aryl-piperazines in 1-72% isolated yields for the process. The scope of iron-assisted SNAr reactions on solid phase was investigated, and reactions of representative nucleophiles from groups VI (O, S, and Se) and V (N and P) of the periodic table were examined. Reactions of resin-bound iron arene complexes with phenylselenide and aniline do not occur; substitution reactions with sodium alkoxides give only modest yields.

IT 453559-54-1D, Merrifield resin-bound 453559-55-2D, Merrifield resin-bound

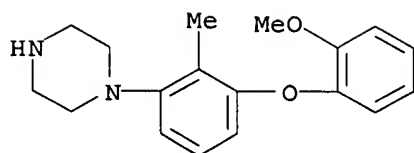
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of a library of arylpiperazines and aryl-1,4-diazepanes on solid phase using the nucleophilic aromatic substitution reactions of resin-bound iron arene complexes as the key steps)

RN 453559-54-1 HCAPLUS

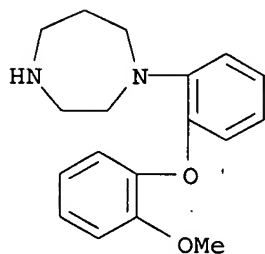
CN Piperazine, 1-[3-(2-methoxyphenoxy)-2-methylphenyl]- (9CI) (CA INDEX

NAME)



RN 453559-55-2 HCAPLUS

CN 1H-1,4-Diazepine, hexahydro-1-[2-(2-methoxyphenoxy)phenyl]- (9CI) (CA INDEX NAME)



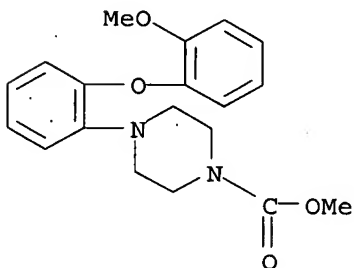
IT 453559-84-7P 453559-87-0P 453559-88-1P

453559-89-2P 453559-90-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of a library of arylpiperazines and aryl-1,4-diazepanes on solid phase using the nucleophilic aromatic substitution reactions of resin-bound iron arene complexes as the key steps)

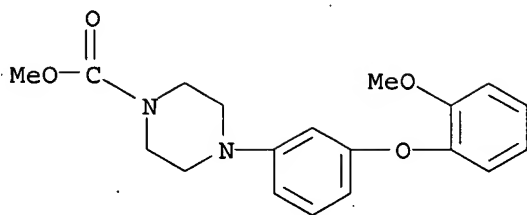
RN 453559-84-7 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(2-methoxyphenoxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



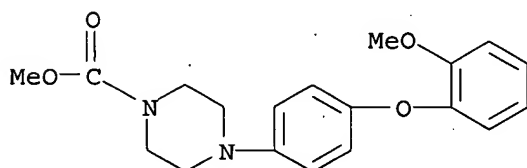
RN 453559-87-0 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[3-(2-methoxyphenoxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



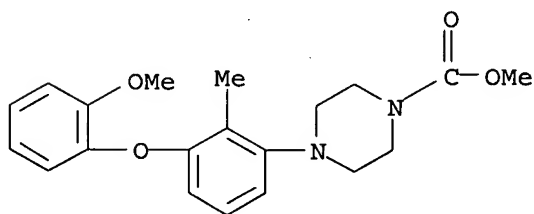
RN 453559-88-1 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2-methoxyphenoxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



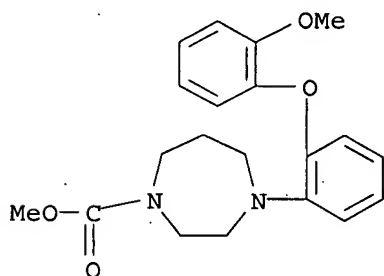
RN 453559-89-2 HCAPLUS

CN 1-Piperazinecarboxylic acid, 4-[3-(2-methoxyphenoxy)-2-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 453559-90-5 HCAPLUS

CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[2-(2-methoxyphenoxy)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

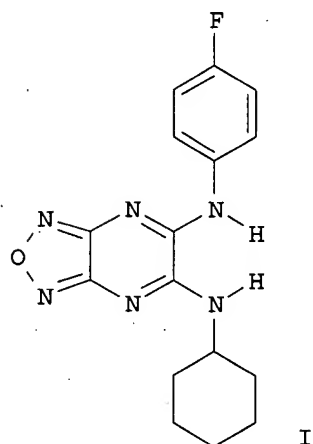
L17 ANSWER 24 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:456633 HCAPLUS

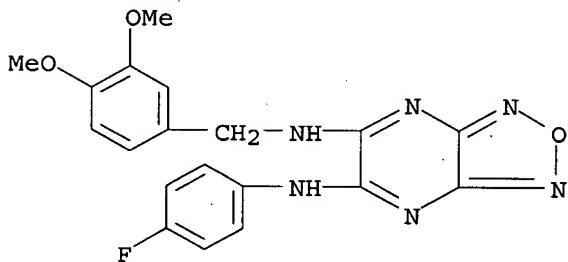
DOCUMENT NUMBER: 137:169485

TITLE: Solid-phase versus solution
synthesis of asymmetrically disubstituted

AUTHOR(S): furazano[3,4-b]pyrazines
 Fernandez, E.; Garcia-Ochoa, S.; Huss, S.; Mallo, A.;
 Bueno, J. M.; Micheli, F.; Paio, A.; Piga, E.;
 Zarantonello, P.
 CORPORATE SOURCE: GlaxoSmithKline S.A. P.T.M., Madrid, E-28760, Spain
 SOURCE: Tetrahedron Letters (2002), 43(27),
 4741-4745
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:169485
 GI



AB Herein we describe a straightforward solid-phase
 synthesis directed towards the preparation of families of asym. disubstituted
 furazano[3,4-b]pyrazines, e.g., I, by stepwise displacement of the two
 chlorine atoms in 5,6-dichlorofurazano[3,4-b]pyrazine by
 nucleophiles. This synthesis has avoided selectivity problems
 found in solution chemical
 IT 448242-59-9P
 RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP
 (Preparation)
 (preparation of asym. disubstituted furazano[3,4-b]pyrazine combinatorial
 libraries via solid phase synthesis)
 RN 448242-59-9 HCAPLUS
 CN [1,2,5]Oxadiazolo[3,4-b]pyrazinediamine, N-[(3,4-dimethoxyphenyl)methyl]-
 N'-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

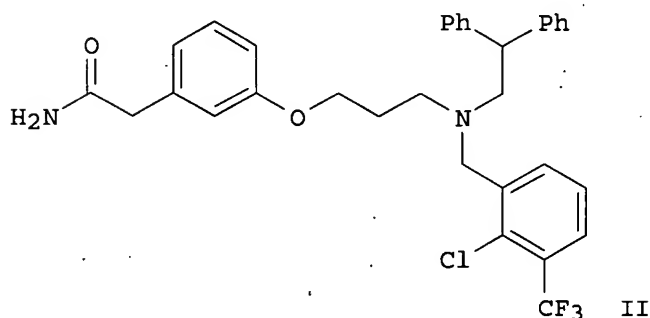
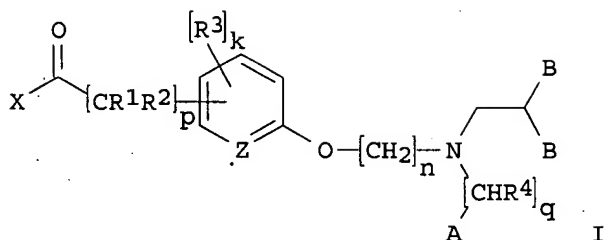


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 25 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:240713 HCAPLUS
 DOCUMENT NUMBER: 136:294650
 TITLE: Preparation of substituted phenylacetamides and
 benzamides as agonists for Liver X receptors (LXR)
 INVENTOR(S): Collins, Jon Loren; Fivush, Adam M.; Maloney, Patrick
 Reed; Stewart, Eugene L.; Willson, Timothy Mark
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK
 SOURCE: PCT Int. Appl., 118 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002024632	A2	20020328	WO 2001-US27622	20010906 <--
WO 2002024632	A3	20020711		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002011216	A5	20020402	AU 2002-11216	20010906 <--
EP 1318976	A2	20030618	EP 2001-979230	20010906 <--
EP 1318976	B1	20041124		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004509161	T	20040325	JP 2002-528647	20010906 <--
AT 283253	T	20041215	AT 2001-979230	20010906 <--
ES 2233700	T3	20050616	ES 2001-1979230	20010906
US 2004072868	A1	20040415	US 2003-380932	20030318 <--
US 2005282908	A1	20051222	US 2005-154852	20050616
PRIORITY APPLN. INFO.:				
			US 2000-233144P	P 20000918
			WO 2001-US27622	W 20010906
			US 2003-380932	A1 20030318
OTHER SOURCE(S): MARPAT 136:294650				
GI				



AB The title compds. [I; X = OH, NH₂; p = 0-6; R₁, R₂ = H, alkyl, alkoxy, thioalkyl; Z = CH, N; when Z = CH, k = 0-4; when Z = N, k = 0-3; R₃ = halo, OH, alkyl, etc.; n = 2-8; q = 0-1; R₄ = H, alkyl, alkenyl, alkenyloxy; A = cycloalkyl, aryl, 4-8 membered heterocycle, 5-6 membered heteroaryl; B = cycloalkyl, aryl] and their pharmaceutically acceptable salts, useful for the prevention or treatment of an LXR mediated disease and condition such as cardiovascular disease and atherosclerosis (no biol. data given), were prepared E.g., a solid phase synthesis of II was given.

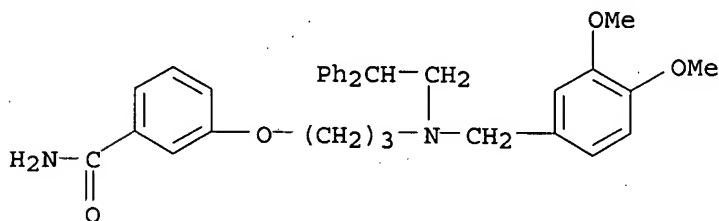
IT 405911-96-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted phenylacetamides and benzamides as agonists for Liver X receptors (LXR))

RN 405911-96-8 HCAPLUS

CN Benzamide, 3-[3-[[[(3,4-dimethoxyphenyl)methyl](2,2-diphenylethyl)amino]propoxy]- (9CI) (CA INDEX NAME)



L17 ANSWER 26 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:97955 HCAPLUS

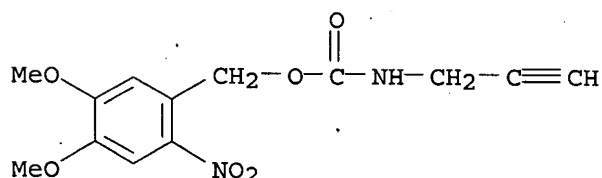
DOCUMENT NUMBER: 136:402007

TITLE: The use of Sonogashira coupling for the synthesis of modified uracil peptide nucleic acid

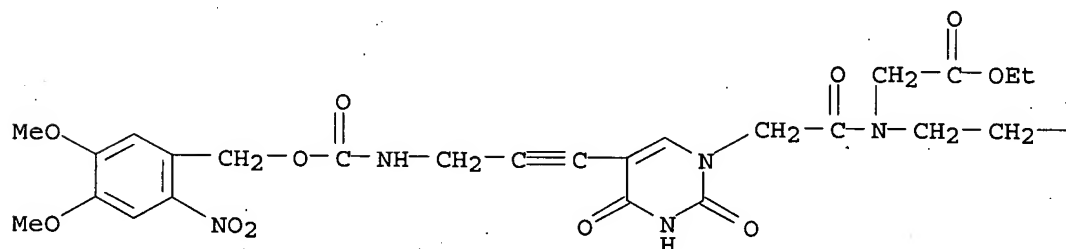
AUTHOR(S): Hudson, Robert H. E.; Li, Ge; Tse, Joseph
 CORPORATE SOURCE: Department of Chemistry, The University of Western
 Ontario, London, ON, N6A 5B7, Can.
 SOURCE: Tetrahedron Letters (2002), 43(8), 1381-1386
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:402007

AB Palladium-catalyzed Sonogashira coupling has been shown to be compatible with PNA monomers as illustrated by the reaction of 5-iodouracil peptide nucleic acid monomer (IU-PNA) with several terminal alkynes. These reactions have been performed in the solution phase and with IU-PNA linked to an insol. polymer support. The results presented herein show that while the isolated yields from the solution phase chemical are modest (38-53%), the yields of the resin-bound coupling reactions are essentially quant., at the monomer level. A selection of alkynes was used to install various addnl. functionality on the uracil nucleobase. Examples of a hydroxyl, protected thiol and protected amino group are given. Further, an example of derivatization of a resin-bound oligomer with a single IU insert is given.

IT 431042-66-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of PNAs containing a modified uracil using Sonogashira coupling reaction in liquid or solid-phase synthesis)
 RN 431042-66-9 HCAPLUS
 CN Carbamic acid, 2-propynyl-, (4,5-dimethoxy-2-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

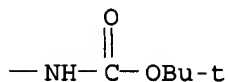


IT 668474-58-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of PNAs containing a modified uracil using Sonogashira coupling reaction in liquid or solid-phase synthesis)
 RN 668474-58-6 HCAPLUS
 CN Glycine, N-[[5-[3-[[[(4,5-dimethoxy-2-nitrophenyl)methoxy]carbonyl]amino]-1-propynyl]-3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl]acetyl]-N-[2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



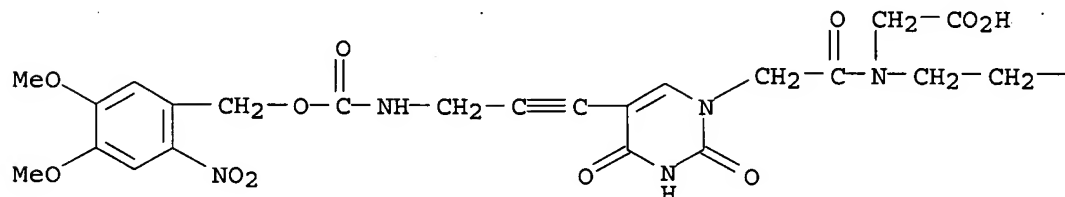
PAGE 1-A

PAGE 1-B

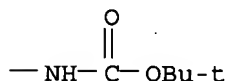


IT 431042-71-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of PNAs containing a modified uracil using Sonogashira coupling
 reaction in liquid or solid-phase synthesis)
 RN 431042-71-6 HCAPLUS
 CN Glycine, N-[[5-[3-[[[(4,5-dimethoxy-2-nitrophenyl)methoxy]carbonyl]amino]-
 1-propynyl]-3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl]acetyl]-N-[2-[[[(1,1-
 dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)

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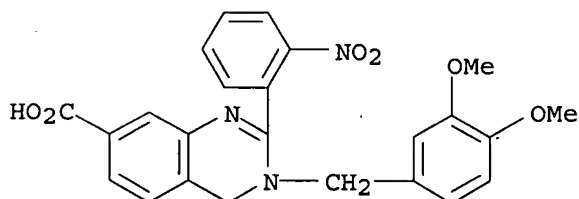
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 27 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2001:818348 HCAPLUS
 DOCUMENT NUMBER: 136:279410
 TITLE: Solid-phase synthesis of
 3,4-dihydroquinazoline derivatives
 AUTHOR(S): Zhang, Jinfang; Barker, Julie; Lou, Boliang; Saneii,
 Hossain
 CORPORATE SOURCE: LLC, Department of Chemistry, Advanced SynTech,
 Louisville, KY, 40299, USA
 SOURCE: Tetrahedron Letters (2001), 42(48),
 8405-8408
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:279410
 AB A novel method for solid-phase synthesis of
 dihydroquinazoline derivs. is presented. Polymer-bound
 4-bromomethyl-3-nitrobenzoate and the corresponding amide were used as
 versatile precursors that undergo nucleophilic displacement with
 amines followed by reduction and cyclocondensation reactions to afford
 structurally diverse dihydroquinazolines with excellent yield and purity.
 IT 405922-54-5P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(solid-phase synthesis of 3,4-dihydroquinazoline derivs.)

RN 405922-54-5 HCAPLUS

CN 7-Quinazolinecarboxylic acid, 3-[(3,4-dimethoxyphenyl)methyl]-3,4-dihydro-2-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 28 OF 28 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:612010 HCAPLUS

DOCUMENT NUMBER: 135:371939

TITLE: Parallel solid-phase synthesis of nucleoside phosphoramidate libraries

AUTHOR(S): Jin, Y.; Chen, X.; Cote, M.-E.; Roland, A.; Korba, B.; Mounir, S.; Iyer, R. P.

CORPORATE SOURCE: Origenix Technologies Inc., Laval, QC, H7V 4A9, Can.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(16), 2057-2060

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:371939

AB Combinatorial chemical is playing an increasingly prominent role in the process of drug discovery. A nucleic acid-based (NAB) scaffold can be engineered to create functional group and topol. diversity in a library. Described herein is the parallel solid-phase synthesis of combinatorial libraries of nucleoside phosphoramidates, and the first evaluation of antiviral activity against hepatitis B virus (HBV).

IT 374591-56-7P

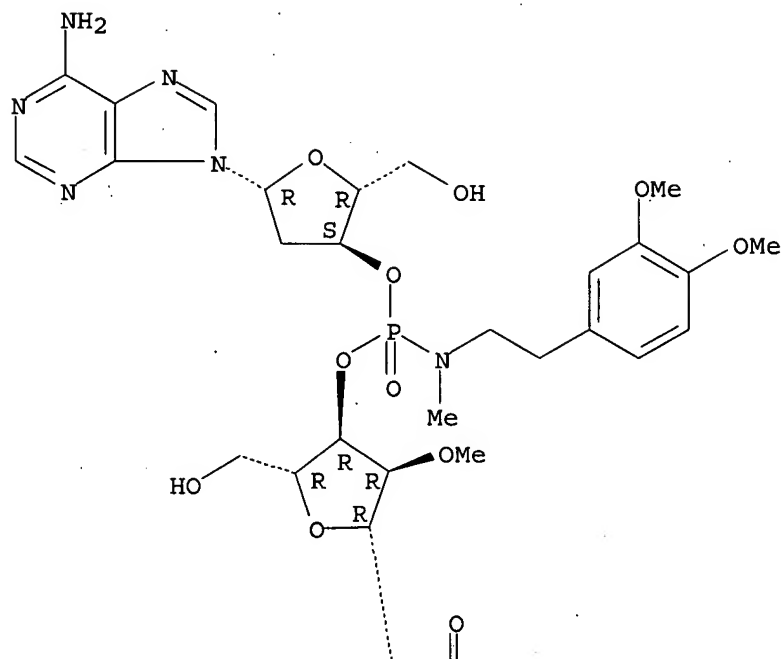
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(parallel solid-phase synthesis of nucleoside phosphoramidate combinatorial libraries)

RN 374591-56-7 HCAPLUS

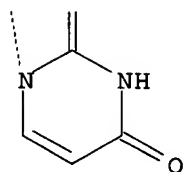
CN Adenosine, P-deoxy-P-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-2'-O-methyluridylyl-(3'→3')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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REFERENCE COUNT:

13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
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